

Propane, 1,1'-[ethylidenebis(oxy)]bis[2-methyl-

Other names:	1,1'-[ethylidenebis(oxy)]bis[2-methylpropane] 2,5,8-Trimethyl-4,6-dioxanonane Acetaldehyde, diisobutyl acetal Diisobutyl acetal Ethane, 1,1-diisobutyloxy Ethylene glycol diisobutyl ether Propane, 1,1'-[ethylidenebis(oxy)]bis*2-methyl-
Inchi:	InChI=1S/C10H22O2/c1-8(2)6-11-10(5)12-7-9(3)4/h8-10H,6-7H2,1-5H3
InchiKey:	KIELJSVPUISYCI-UHFFFAOYSA-N
Formula:	C10H22O2
SMILES:	CC(C)COC(C)OCC(C)C
Mol. weight [g/mol]:	174.28
CAS:	5669-09-0

Physical Properties

Property code	Value	Unit	Source
gf	-184.00	kJ/mol	Joback Method
hf	-530.01	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	41.51	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.678		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	959.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	949.00		NIST Webbook
ripol	1072.00		NIST Webbook
ripol	1072.00		NIST Webbook
tb	449.00 ± 4.00	K	NIST Webbook
tc	644.52	K	Joback Method
tf	201.92	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.76	J/mol×K	644.52	Joback Method
cpg	369.61	J/mol×K	471.72	Joback Method
cpg	385.27	J/mol×K	500.52	Joback Method
cpg	400.40	J/mol×K	529.32	Joback Method
cpg	415.02	J/mol×K	558.12	Joback Method
cpg	429.12	J/mol×K	586.92	Joback Method
cpg	442.70	J/mol×K	615.72	Joback Method
dvisc	0.0001458	Pa×s	471.72	Joback Method
dvisc	0.0139337	Pa×s	201.92	Joback Method
dvisc	0.0032621	Pa×s	246.89	Joback Method
dvisc	0.0011946	Pa×s	291.85	Joback Method
dvisc	0.0005721	Pa×s	336.82	Joback Method
dvisc	0.0003258	Pa×s	381.79	Joback Method
dvisc	0.0002090	Pa×s	426.75	Joback Method
hvapt	46.10	kJ/mol	396.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.16009e+01
Coeff. B	-3.13326e+03
Coeff. C	-6.47070e+01
Temperature range (K), min.	297.98
Temperature range (K), max.	562.88

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5669090&Units=SI>

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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