

Butane, 1-(ethenyloxy)-3-methyl-

Other names:	Vinylisopentyl ether
Inchi:	InChI=1S/C7H14O/c1-4-8-6-5-7(2)3/h4,7H,1,5-6H2,2-3H3
InchiKey:	QIUCYKBVFAPWRR-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	C=COCCC(C)C
Mol. weight [g/mol]:	114.19
CAS:	39782-38-2

Physical Properties

Property code	Value	Unit	Source
chl	-4490.00 ± 13.00	kJ/mol	NIST Webbook
gf	-11.54	kJ/mol	Joback Method
hf	-199.88	kJ/mol	Joback Method
hfus	10.27	kJ/mol	Joback Method
hvap	32.53	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.193		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
tb	378.22	K	Joback Method
tc	549.86	K	Joback Method
tf	174.12	K	Joback Method
vc	0.420	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.01	J/mol×K	378.22	Joback Method
cpg	215.27	J/mol×K	406.83	Joback Method
cpg	226.16	J/mol×K	435.43	Joback Method
cpg	236.67	J/mol×K	464.04	Joback Method
cpg	246.82	J/mol×K	492.64	Joback Method
cpg	256.61	J/mol×K	521.25	Joback Method
cpg	266.03	J/mol×K	549.86	Joback Method

dvisc	0.0056980	Paxs	174.12	Joback Method
dvisc	0.0020983	Paxs	208.14	Joback Method
dvisc	0.0010231	Paxs	242.15	Joback Method
dvisc	0.0005954	Paxs	276.17	Joback Method
dvisc	0.0003902	Paxs	310.19	Joback Method
dvisc	0.0002780	Paxs	344.20	Joback Method
dvisc	0.0002105	Paxs	378.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39782382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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