

Diamyl oxalate

Inchi:	InChI=1S/C12H22O4/c1-3-5-7-9-15-11(13)12(14)16-10-8-6-4-2/h3-10H2,1-2H3
InchiKey:	XAHVPYNDLCTDTE-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CCCCCOC(=O)C(=O)OCCCCC
Mol. weight [g/mol]:	230.30

Physical Properties

Property code	Value	Unit	Source
gf	-417.68	kJ/mol	Joback Method
hf	-780.61	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.453		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1518.00		NIST Webbook
tb	626.54	K	Joback Method
tc	803.91	K	Joback Method
tf	369.32	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.96	J/molxK	626.54	Joback Method
cpg	530.51	J/molxK	656.10	Joback Method
cpg	544.42	J/molxK	685.66	Joback Method
cpg	557.71	J/molxK	715.23	Joback Method
cpg	570.37	J/molxK	744.79	Joback Method
cpg	582.39	J/molxK	774.35	Joback Method
cpg	593.78	J/molxK	803.91	Joback Method
dvisc	0.0017118	Paxs	369.32	Joback Method
dvisc	0.0009273	Paxs	412.19	Joback Method

dvisc	0.0005638	Paxs	455.06	Joback Method
dvisc	0.0003735	Paxs	497.93	Joback Method
dvisc	0.0002641	Paxs	540.80	Joback Method
dvisc	0.0001965	Paxs	583.67	Joback Method
dvisc	0.0001522	Paxs	626.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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