

Diethylmalonic acid, 2-ethoxyethyl ethyl ester

Inchi:	InChI=1S/C13H24O5/c1-5-13(6-2,11(14)17-8-4)12(15)18-10-9-16-7-3/h5-10H2,1-4H3
InchiKey:	BUGUAXBWWKSCSM-UHFFFAOYSA-N
Formula:	C13H24O5
SMILES:	CCOCCOC(=O)C(CC)(CC)C(=O)OCC
Mol. weight [g/mol]:	260.33

Physical Properties

Property code	Value	Unit	Source
gf	-511.42	kJ/mol	Joback Method
hf	-942.22	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	63.96	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.936		Crippen Method
mcvol	214.780	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinsol	1504.00		NIST Webbook
tb	668.61	K	Joback Method
tc	852.22	K	Joback Method
tf	405.24	K	Joback Method
vc	0.819	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.16	J/molxK	668.61	Joback Method
cpg	668.26	J/molxK	821.62	Joback Method
cpg	655.98	J/molxK	791.02	Joback Method
cpg	642.93	J/molxK	760.42	Joback Method
cpg	629.11	J/molxK	729.81	Joback Method
cpg	614.53	J/molxK	699.21	Joback Method
cpg	679.79	J/molxK	852.22	Joback Method
dvisc	0.0000894	Paxs	668.61	Joback Method
dvisc	0.0001180	Paxs	624.72	Joback Method

dvisc	0.0001622	Paxs	580.82	Joback Method
dvisc	0.0002350	Paxs	536.92	Joback Method
dvisc	0.0003637	Paxs	493.03	Joback Method
dvisc	0.0006130	Paxs	449.13	Joback Method
dvisc	0.0011570	Paxs	405.24	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370605&Units=SI

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
mcvol:	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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