

Diethylmalonic acid, 2-ethoxyethyl tetradecyl ester

Inchi:	InChI=1S/C25H48O5/c1-5-9-10-11-12-13-14-15-16-17-18-19-20-29-23(26)25(6-2,7-3)24
InchiKey:	ASJYEEPEVGNMFX-UHFFFAOYSA-N
Formula:	C25H48O5
SMILES:	CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCOCC
Mol. weight [g/mol]:	428.65

Physical Properties

Property code	Value	Unit	Source
gf	-410.38	kJ/mol	Joback Method
hf	-1189.90	kJ/mol	Joback Method
hfus	59.85	kJ/mol	Joback Method
hvap	90.67	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.617		Crippen Method
mcvol	383.860	ml/mol	McGowan Method
pc	805.25	kPa	Joback Method
rinpol	2641.00		NIST Webbook
tb	943.17	K	Joback Method
tc	1157.86	K	Joback Method
tf	540.48	K	Joback Method
vc	1.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.06	J/molxK	943.17	Joback Method
cpg	1397.72	J/molxK	1122.08	Joback Method
cpg	1383.78	J/molxK	1086.30	Joback Method
cpg	1368.39	J/molxK	1050.52	Joback Method
cpg	1351.51	J/molxK	1014.73	Joback Method
cpg	1333.08	J/molxK	978.95	Joback Method
cpg	1410.26	J/molxK	1157.86	Joback Method
dvisc	0.0000142	Paxs	943.17	Joback Method
dvisc	0.0000193	Paxs	876.06	Joback Method

dvisc	0.0000276	Paxs	808.94	Joback Method
dvisc	0.0000420	Paxs	741.83	Joback Method
dvisc	0.0000696	Paxs	674.71	Joback Method
dvisc	0.0001290	Paxs	607.60	Joback Method
dvisc	0.0002783	Paxs	540.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370615&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

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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