Diethylmalonic acid, 2-ethoxylethyl propyl ester

Inchi: InChI=1S/C14H26O5/c1-5-9-18-12(15)14(6-2,7-3)13(16)19-11-10-17-8-4/h5-11H2,1-4H3

InchiKey: DBIBEKPRHYHVGE-UHFFFAOYSA-N

Formula: C14H26O5

SMILES: CCCOC(=O)C(CC)(CC)C(=O)OCCOCC

Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
gf	-503.00	kJ/mol	Joback Method
hf	-962.86	kJ/mol	Joback Method
hfus	31.36	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.326		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	1586.00		NIST Webbook
tb	691.49	K	Joback Method
tc	874.22	K	Joback Method
tf	416.51	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.43	J/mol×K	691.49	Joback Method
cpg	669.24	J/mol×K	721.94	Joback Method
cpg	684.23	J/mol×K	752.40	Joback Method
cpg	698.40	J/mol×K	782.85	Joback Method
cpg	711.78	J/mol×K	813.31	Joback Method
cpg	724.35	J/mol×K	843.76	Joback Method
cpg	736.14	J/mol×K	874.22	Joback Method
dvisc	0.0010508	Pa×s	416.51	Joback Method
dvisc	0.0005490	Pa×s	462.34	Joback Method

dvisc	0.0003225	Pa×s	508.17	Joback Method
dvisc	0.0002068	Pa×s	554.00	Joback Method
dvisc	0.0001420	Pa×s	599.83	Joback Method
dvisc	0.0001028	Pa×s	645.66	Joback Method
dvisc	0.0000777	Pa×s	691.49	Joback Method

Sources

Crippen Method: 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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370606&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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