Diethylmalonic acid, heptyl pentadecyl ester

Inchi: InChI=1S/C29H56O4/c1-5-9-11-13-14-15-16-17-18-19-20-22-24-26-33-28(31)29(7-3,8-4
InchiKey: VXTPZXPYJXZQPC-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCC
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-271.70	kJ/mol	Joback Method
hf	-1140.24	kJ/mol	Joback Method
hfus	69.03	kJ/mol	Joback Method
hvap	97.16	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.941		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	660.51	kPa	Joback Method
rinpol	2972.00		NIST Webbook
tb	1012.27	K	Joback Method
tc	1256.59	K	Joback Method
tf	563.33	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.29	J/mol×K	1012.27	Joback Method
cpg	1562.26	J/mol×K	1052.99	Joback Method
cpg	1583.28	J/mol×K	1093.71	Joback Method
cpg	1602.46	J/mol×K	1134.43	Joback Method
cpg	1619.92	J/mol×K	1175.15	Joback Method
cpg	1635.76	J/mol×K	1215.87	Joback Method
cpg	1650.11	J/mol×K	1256.59	Joback Method
dvisc	0.0002393	Pa×s	563.33	Joback Method
dvisc	0.0001037	Pa×s	638.15	Joback Method

dvisc	0.0000535	Pa×s	712.98	Joback Method
dvisc	0.0000313	Pa×s	787.80	Joback Method
dvisc	0.0000201	Pa×s	862.62	Joback Method
dvisc	0.0000139	Pa×s	937.45	Joback Method
dvisc	0.0000101	Pa×s	1012.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369523&Units=SI
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

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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