

Diethylmalonic acid, octadecyl 2-octyl ester

Inchi: InChI=1S/C33H64O4/c1-6-10-12-14-15-16-17-18-19-20-21-22-23-24-25-27-29-36-31(34)
InchiKey: SBJJIHPRJNSUFT-UHFFFAOYSA-N
Formula: C33H64O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CCCCC
Mol. weight [g/mol]: 524.86

Physical Properties

Property code	Value	Unit	Source
gf	-240.46	kJ/mol	Joback Method
hf	-1228.08	kJ/mol	Joback Method
hfus	75.86	kJ/mol	Joback Method
hvap	105.68	kJ/mol	Joback Method
log10ws	-11.23		Crippen Method
logp	10.500		Crippen Method
mcvol	490.710	ml/mol	McGowan Method
pc	549.23	kPa	Joback Method
rinpol	3270.00		NIST Webbook
rinpol	3270.00		NIST Webbook
tb	1103.35	K	Joback Method
tc	1402.99	K	Joback Method
tf	593.41	K	Joback Method
vc	1.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1802.93	J/molxK	1103.35	Joback Method
cpg	1829.08	J/molxK	1153.29	Joback Method
cpg	1852.42	J/molxK	1203.23	Joback Method
cpg	1873.21	J/molxK	1253.17	Joback Method
cpg	1891.68	J/molxK	1303.11	Joback Method
cpg	1908.08	J/molxK	1353.05	Joback Method
cpg	1922.64	J/molxK	1402.99	Joback Method
dvisc	0.0001480	Paxs	593.41	Joback Method

dvisc	0.0000581	Paxs	678.40	Joback Method
dvisc	0.0000281	Paxs	763.39	Joback Method
dvisc	0.0000157	Paxs	848.38	Joback Method
dvisc	0.0000097	Paxs	933.37	Joback Method
dvisc	0.0000066	Paxs	1018.36	Joback Method
dvisc	0.0000047	Paxs	1103.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369378&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
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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