

Diethylmalonic acid, 3,7-dimethyloctyl hexadecyl ester

Inchi:	InChI=1S/C33H64O4/c1-7-10-11-12-13-14-15-16-17-18-19-20-21-22-27-36-31(34)33(8-2
InchiKey:	SBIPXPRVASVWRY-UHFFFAOYSA-N
Formula:	C33H64O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	524.86

Physical Properties

Property code	Value	Unit	Source
gf	-242.90	kJ/mol	Joback Method
hf	-1233.36	kJ/mol	Joback Method
hfus	72.34	kJ/mol	Joback Method
hvap	105.29	kJ/mol	Joback Method
log10ws	-10.64		Crippen Method
logp	10.213		Crippen Method
mvol	490.710	ml/mol	McGowan Method
pc	551.30	kPa	Joback Method
rinpol	3219.00		NIST Webbook
rinpol	3219.00		NIST Webbook
tb	1102.91	K	Joback Method
tc	1398.00	K	Joback Method
tf	578.41	K	Joback Method
vc	1.909	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1802.97	J/molxK	1102.91	Joback Method
cpg	1828.61	J/molxK	1152.09	Joback Method
cpg	1851.50	J/molxK	1201.27	Joback Method
cpg	1871.88	J/molxK	1250.46	Joback Method
cpg	1889.98	J/molxK	1299.64	Joback Method
cpg	1906.02	J/molxK	1348.82	Joback Method
cpg	1920.24	J/molxK	1398.00	Joback Method
dvisc	0.0001678	Paxs	578.41	Joback Method

dvisc	0.0000608	Paxs	665.83	Joback Method
dvisc	0.0000279	Paxs	753.24	Joback Method
dvisc	0.0000151	Paxs	840.66	Joback Method
dvisc	0.0000091	Paxs	928.08	Joback Method
dvisc	0.0000060	Paxs	1015.49	Joback Method
dvisc	0.0000043	Paxs	1102.91	Joback Method

Sources

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=U369414&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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