

Diethylmalonic acid, hexadecyl 3-methylbutyl ester

Inchi:	InChI=1S/C28H54O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-21-23-31-26(29)28(7-2,
InchiKey:	IQJLLXFDNDMQW-UHFFFAOYSA-N
Formula:	C28H54O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)C
Mol. weight [g/mol]:	454.73

Physical Properties

Property code	Value	Unit	Source
gf	-282.56	kJ/mol	Joback Method
hf	-1124.88	kJ/mol	Joback Method
hfus	62.91	kJ/mol	Joback Method
hvap	94.55	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	8.407		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	697.28	kPa	Joback Method
rinsol	2821.00		NIST Webbook
tb	988.95	K	Joback Method
tc	1220.27	K	Joback Method
tf	537.06	K	Joback Method
vc	1.635	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.43	J/molxK	988.95	Joback Method
cpg	1496.42	J/molxK	1027.50	Joback Method
cpg	1516.64	J/molxK	1066.06	Joback Method
cpg	1535.17	J/molxK	1104.61	Joback Method
cpg	1552.12	J/molxK	1143.16	Joback Method
cpg	1567.57	J/molxK	1181.71	Joback Method
cpg	1581.62	J/molxK	1220.27	Joback Method
dvisc	0.0003161	Paxs	537.06	Joback Method
dvisc	0.0001276	Paxs	612.38	Joback Method

dvisc	0.0000628	Paxs	687.69	Joback Method
dvisc	0.0000356	Paxs	763.00	Joback Method
dvisc	0.0000223	Paxs	838.32	Joback Method
dvisc	0.0000151	Paxs	913.63	Joback Method
dvisc	0.0000109	Paxs	988.95	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=U369395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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