

Diethylmalonic acid, heptadecyl 2-hexyl ester

Inchi:	InChI=1S/C30H58O4/c1-6-10-12-13-14-15-16-17-18-19-20-21-22-23-24-26-33-28(31)30
InchiKey:	BFECJKPYAHECCT-UHFFFAOYSA-N
Formula:	C30H58O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CCCC
Mol. weight [g/mol]:	482.78

Physical Properties

Property code	Value	Unit	Source
gf	-265.72	kJ/mol	Joback Method
hf	-1166.16	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	99.00	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	9.329		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	631.61	kPa	Joback Method
rinpol	2985.00		NIST Webbook
tb	1034.71	K	Joback Method
tc	1288.59	K	Joback Method
tf	559.60	K	Joback Method
vc	1.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.99	J/molxK	1034.71	Joback Method
cpg	1702.40	J/molxK	1246.28	Joback Method
cpg	1686.61	J/molxK	1203.97	Joback Method
cpg	1669.10	J/molxK	1161.65	Joback Method
cpg	1649.75	J/molxK	1119.34	Joback Method
cpg	1628.42	J/molxK	1077.02	Joback Method
cpg	1716.62	J/molxK	1288.59	Joback Method
dvisc	0.0000078	Paxs	1034.71	Joback Method
dvisc	0.0000109	Paxs	955.52	Joback Method

dvisc	0.0000161	Paxs	876.34	Joback Method
dvisc	0.0000257	Paxs	797.15	Joback Method
dvisc	0.0000457	Paxs	717.97	Joback Method
dvisc	0.0000935	Paxs	638.78	Joback Method
dvisc	0.0002345	Paxs	559.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	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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