

Diethylmalonic acid, heptadecyl heptyl ester

Inchi:	InChI=1S/C31H60O4/c1-5-9-11-13-14-15-16-17-18-19-20-21-22-24-26-28-35-30(33)31(7
InchiKey:	QGEKIQJTHZUEKM-UHFFFAOYSA-N
Formula:	C31H60O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCC
Mol. weight [g/mol]:	496.81

Physical Properties

Property code	Value	Unit	Source
gf	-254.86	kJ/mol	Joback Method
hf	-1181.52	kJ/mol	Joback Method
hfus	74.21	kJ/mol	Joback Method
hvap	101.62	kJ/mol	Joback Method
log10ws	-10.28		Crippen Method
logp	9.721		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	599.85	kPa	Joback Method
rinpol	3171.00		NIST Webbook
tb	1058.03	K	Joback Method
tc	1328.97	K	Joback Method
tf	585.87	K	Joback Method
vc	1.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.57	J/molxK	1058.03	Joback Method
cpg	1772.07	J/molxK	1283.81	Joback Method
cpg	1755.80	J/molxK	1238.66	Joback Method
cpg	1737.68	J/molxK	1193.50	Joback Method
cpg	1717.54	J/molxK	1148.34	Joback Method
cpg	1695.23	J/molxK	1103.19	Joback Method
cpg	1786.66	J/molxK	1328.97	Joback Method
dvisc	0.0000072	Paxs	1058.03	Joback Method
dvisc	0.0000100	Paxs	979.34	Joback Method

dvisc	0.0000145	Paxs	900.64	Joback Method
dvisc	0.0000227	Paxs	821.95	Joback Method
dvisc	0.0000390	Paxs	743.26	Joback Method
dvisc	0.0000763	Paxs	664.56	Joback Method
dvisc	0.0001785	Paxs	585.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369525&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
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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