

Diethylmalonic acid, butyl octadecyl ester

Inchi:	InChI=1S/C29H56O4/c1-5-9-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26-33-28(31)2
InchiKey:	VXHCTDUEYBIKCG-UHFFFAOYSA-N
Formula:	C29H56O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCC
Mol. weight [g/mol]:	468.75

Physical Properties

Property code	Value	Unit	Source
gf	-271.70	kJ/mol	Joback Method
hf	-1140.24	kJ/mol	Joback Method
hfus	69.03	kJ/mol	Joback Method
hvap	97.16	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.941		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	660.51	kPa	Joback Method
rinsol	3003.00		NIST Webbook
tb	1012.27	K	Joback Method
tc	1256.59	K	Joback Method
tf	563.33	K	Joback Method
vc	1.696	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.29	J/molxK	1012.27	Joback Method
cpg	1635.76	J/molxK	1215.87	Joback Method
cpg	1619.92	J/molxK	1175.15	Joback Method
cpg	1602.46	J/molxK	1134.43	Joback Method
cpg	1583.28	J/molxK	1093.71	Joback Method
cpg	1562.26	J/molxK	1052.99	Joback Method
cpg	1650.11	J/molxK	1256.59	Joback Method
dvisc	0.0000101	Paxs	1012.27	Joback Method
dvisc	0.0000139	Paxs	937.45	Joback Method

dvisc	0.0000201	Paxs	862.62	Joback Method
dvisc	0.0000313	Paxs	787.80	Joback Method
dvisc	0.0000535	Paxs	712.98	Joback Method
dvisc	0.0001037	Paxs	638.15	Joback Method
dvisc	0.0002393	Paxs	563.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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