

Diethylmalonic acid, 3,7-dimethyloctyl dodecyl ester

Inchi:	InChI=1S/C29H56O4/c1-7-10-11-12-13-14-15-16-17-18-23-32-27(30)29(8-2,9-3)28(31)3
InchiKey:	NNWYGBVMBWXLAK-UHFFFAOYSA-N
Formula:	C29H56O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	468.75

Physical Properties

Property code	Value	Unit	Source
gf	-276.58	kJ/mol	Joback Method
hf	-1150.80	kJ/mol	Joback Method
hfus	61.98	kJ/mol	Joback Method
hvap	96.39	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	8.653		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	665.97	kPa	Joback Method
rinqol	2806.00		NIST Webbook
tb	1011.39	K	Joback Method
tc	1251.02	K	Joback Method
tf	533.33	K	Joback Method
vc	1.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.80	J/molxK	1011.39	Joback Method
cpg	1562.21	J/molxK	1051.33	Joback Method
cpg	1582.70	J/molxK	1091.27	Joback Method
cpg	1601.39	J/molxK	1131.21	Joback Method
cpg	1618.39	J/molxK	1171.14	Joback Method
cpg	1633.79	J/molxK	1211.08	Joback Method
cpg	1647.71	J/molxK	1251.02	Joback Method
dvisc	0.0003150	Paxs	533.33	Joback Method
dvisc	0.0001161	Paxs	613.01	Joback Method

dvisc	0.0000539	Paxs	692.68	Joback Method
dvisc	0.0000293	Paxs	772.36	Joback Method
dvisc	0.0000178	Paxs	852.04	Joback Method
dvisc	0.0000118	Paxs	931.71	Joback Method
dvisc	0.0000084	Paxs	1011.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369411&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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