

Diethylmalonic acid, decyl 3,7-dimethyloctyl ester

Inchi:	InChI=1S/C27H52O4/c1-7-10-11-12-13-14-15-16-21-30-25(28)27(8-2,9-3)26(29)31-22-2
InchiKey:	BFANIPOQZGCUCF-UHFFFAOYSA-N
Formula:	C27H52O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	440.70

Physical Properties

Property code	Value	Unit	Source
gf	-293.42	kJ/mol	Joback Method
hf	-1109.52	kJ/mol	Joback Method
hfus	56.80	kJ/mol	Joback Method
hvap	91.94	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.872		Crippen Method
mvol	406.170	ml/mol	McGowan Method
pc	737.22	kPa	Joback Method
rinpol	2618.00		NIST Webbook
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tb	965.63	K	Joback Method
tc	1186.37	K	Joback Method
tf	510.79	K	Joback Method
vc	1.573	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.02	J/molxK	965.63	Joback Method
cpg	1500.44	J/molxK	1149.58	Joback Method
cpg	1485.31	J/molxK	1112.79	Joback Method
cpg	1468.78	J/molxK	1076.00	Joback Method
cpg	1450.77	J/molxK	1039.21	Joback Method
cpg	1431.21	J/molxK	1002.42	Joback Method
cpg	1514.25	J/molxK	1186.37	Joback Method
dvisc	0.0000117	Paxs	965.63	Joback Method

dvisc	0.0000165	Paxs	889.82	Joback Method
dvisc	0.0000248	Paxs	814.02	Joback Method
dvisc	0.0000406	Paxs	738.21	Joback Method
dvisc	0.0000744	Paxs	662.40	Joback Method
dvisc	0.0001593	Paxs	586.60	Joback Method
dvisc	0.0004279	Paxs	510.79	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=U369409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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