

Diethylmalonic acid, 3,7-dimethyloctyl isobutyl ester

Inchi:	InChI=1S/C21H40O4/c1-8-21(9-2,20(23)25-15-17(5)6)19(22)24-14-13-18(7)12-10-11-16
InchiKey:	FDLIFGVJKZJDAD-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CCC(CC)(C(=O)O)CCCC(C)CCCC(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	356.54

Physical Properties

Property code	Value	Unit	Source
gf	-346.38	kJ/mol	Joback Method
hf	-990.96	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	78.19	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.388		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1041.25	kPa	Joback Method
rinsol	2018.00		NIST Webbook
tb	827.91	K	Joback Method
tc	1019.21	K	Joback Method
tf	428.17	K	Joback Method
vc	1.230	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.42	J/molxK	827.91	Joback Method
cpg	1115.42	J/molxK	987.33	Joback Method
cpg	1101.01	J/molxK	955.44	Joback Method
cpg	1085.54	J/molxK	923.56	Joback Method
cpg	1068.97	J/molxK	891.68	Joback Method
cpg	1051.28	J/molxK	859.79	Joback Method
cpg	1128.80	J/molxK	1019.21	Joback Method
dvisc	0.0000283	Paxs	827.91	Joback Method
dvisc	0.0000404	Paxs	761.29	Joback Method

dvisc	0.0000618	Paxs	694.66	Joback Method
dvisc	0.0001036	Paxs	628.04	Joback Method
dvisc	0.0001961	Paxs	561.42	Joback Method
dvisc	0.0004409	Paxs	494.79	Joback Method
dvisc	0.0012756	Paxs	428.17	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=U369403&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
mccvol:	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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