Diethylmalonic acid, 3-methylpent-2-yl pentyl ester

Inchi: InChI=1S/C18H34O4/c1-7-11-12-13-21-16(19)18(9-3,10-4)17(20)22-15(6)14(5)8-2/h14-1

InchiKey: PQJAJFVMCVUCDN-UHFFFAOYSA-N

Formula: C18H34O4

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(C)CC

Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-369.20	kJ/mol	Joback Method
hf	-923.76	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	71.90	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.504		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
tb	759.71	K	Joback Method
tc	945.81	K	Joback Method
tf	409.36	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.02	J/mol×K	759.71	Joback Method
cpg	869.92	J/mol×K	790.73	Joback Method
cpg	886.82	J/mol×K	821.74	Joback Method
cpg	902.72	J/mol×K	852.76	Joback Method
cpg	917.67	J/mol×K	883.78	Joback Method
cpg	931.67	J/mol×K	914.80	Joback Method
cpg	944.77	J/mol×K	945.81	Joback Method
dvisc	0.0015357	Pa×s	409.36	Joback Method

dvisc	0.0006044	Pa×s	467.75	Joback Method
dvisc	0.0002925	Pa×s	526.14	Joback Method
dvisc	0.0001637	Pa×s	584.54	Joback Method
dvisc	0.0001018	Pa×s	642.93	Joback Method
dvisc	0.0000685	Pa×s	701.32	Joback Method
dvisc	0.0000490	Pa×s	759.71	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=U369730&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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