Diethylmalonic acid, di(3-methylpentyl) ester

Inchi: InChI=1S/C19H36O4/c1-7-15(5)11-13-22-17(20)19(9-3,10-4)18(21)23-14-12-16(6)8-2/h1
InchiKey: CPDBGTXAVWPFGR-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CCC(C)CCOC(=O)C(CC)(CC)C(=O)OCCC(C)CC
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-360.78	kJ/mol	Joback Method
hf	-944.40	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	74.13	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.752		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	1748.00		NIST Webbook
tb	782.59	K	Joback Method
tc	969.42	K	Joback Method
tf	420.63	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.15	J/mol×K	782.59	Joback Method
cpg	991.84	J/mol×K	938.28	Joback Method
cpg	977.69	J/mol×K	907.14	Joback Method
cpg	962.57	J/mol×K	876.00	Joback Method
cpg	946.47	J/mol×K	844.87	Joback Method
cpg	929.33	J/mol×K	813.73	Joback Method
cpg	1005.05	J/mol×K	969.42	Joback Method
dvisc	0.0000421	Pa×s	782.59	Joback Method
dvisc	0.0000589	Pa×s	722.26	Joback Method

dvisc	0.0000876	Pa×s	661.94	Joback Method
dvisc	0.0001413	Pa×s	601.61	Joback Method
dvisc	0.0002533	Pa×s	541.28	Joback Method
dvisc	0.0005259	Pa×s	480.96	Joback Method
dvisc	0.0013462	Pa×s	420.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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