Diethylmalonic acid, isobutyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C19H36O4/c1-9-19(10-2,16(20)22-12-14(3)4)17(21)23-13-15(5)11-18(6,7)8/h1

InchiKey: SPMNKTXYOIMISB-UHFFFAOYSA-N

Formula: C19H36O4

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-357.94	kJ/mol	Joback Method
hf	-953.15	kJ/mol	Joback Method
hfus	28.67	kJ/mol	Joback Method
hvap	72.83	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.607		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinpol	1790.00		NIST Webbook
tb	779.36	K	Joback Method
tc	971.10	K	Joback Method
tf	423.05	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.49	J/mol×K	779.36	Joback Method
cpg	930.90	J/mol×K	811.32	Joback Method
cpg	948.21	J/mol×K	843.27	Joback Method
cpg	964.46	J/mol×K	875.23	Joback Method
cpg	979.69	J/mol×K	907.19	Joback Method
cpg	993.96	J/mol×K	939.15	Joback Method
cpg	1007.30	J/mol×K	971.10	Joback Method
dvisc	0.0013351	Pa×s	423.05	Joback Method
dvisc	0.0004975	Pa×s	482.43	Joback Method

dvisc	0.0002302	Pa×s	541.82	Joback Method
dvisc	0.0001240	Pa×s	601.20	Joback Method
dvisc	0.0000747	Pa×s	660.59	Joback Method
dvisc	0.0000489	Pa×s	719.98	Joback Method
dvisc	0.0000341	Pa×s	779.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369475&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