Diethylmalonic acid, di(3-methylpent-2-yl) ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-365.66	kJ/mol	Joback Method
hf	-954.96	kJ/mol	Joback Method
hfus	29.03	kJ/mol	Joback Method
hvap	73.35	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.748		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook
tb	781.71	K	Joback Method
tc	972.01	K	Joback Method
tf	390.63	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.12	J/mol×K	781.71	Joback Method
cpg	930.66	J/mol×K	813.43	Joback Method
cpg	948.08	J/mol×K	845.14	Joback Method
cpg	964.43	J/mol×K	876.86	Joback Method
cpg	979.72	J/mol×K	908.58	Joback Method
cpg	994.00	J/mol×K	940.30	Joback Method
cpg	1007.29	J/mol×K	972.01	Joback Method
dvisc	0.0022222	Pa×s	390.63	Joback Method

dvisc	0.0006817	Pa×s	455.81	Joback Method
dvisc	0.0002811	Pa×s	520.99	Joback Method
dvisc	0.0001411	Pa×s	586.17	Joback Method
dvisc	0.0000813	Pa×s	651.35	Joback Method
dvisc	0.0000518	Pa×s	716.53	Joback Method
dvisc	0.0000356	Pa×s	781.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369744&Units=SI

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