Diethylmalonic acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C23H44O4/c1-11-23(12-2,19(24)26-15-17(3)13-21(5,6)7)20(25)27-16-18(4)14-

InchiKey: KRDLTODXEOUAMY-UHFFFAOYSA-N

Formula: C23H44O4

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

Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-321.42	kJ/mol	Joback Method
hf	-1044.46	kJ/mol	Joback Method
hfus	31.61	kJ/mol	Joback Method
hvap	80.44	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	6.024		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	940.37	kPa	Joback Method
rinpol	2063.00		NIST Webbook
tb	867.65	K	Joback Method
tc	1067.87	K	Joback Method
tf	470.55	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.39	J/mol×K	867.65	Joback Method
cpg	1241.96	J/mol×K	1034.50	Joback Method
cpg	1226.96	J/mol×K	1001.13	Joback Method
cpg	1210.98	J/mol×K	967.76	Joback Method
cpg	1193.95	J/mol×K	934.39	Joback Method
cpg	1175.77	J/mol×K	901.02	Joback Method
cpg	1256.06	J/mol×K	1067.87	Joback Method
dvisc	0.0000138	Pa×s	867.65	Joback Method
dvisc	0.0000202	Pa×s	801.47	Joback Method

dvisc	0.0000318	Pa×s	735.28	Joback Method
dvisc	0.0000545	Pa×s	669.10	Joback Method
dvisc	0.0001052	Pa×s	602.92	Joback Method
dvisc	0.0002388	Pa×s	536.73	Joback Method
dvisc	0.0006830	Pa×s	470.55	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=U369491&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