Diethylmalonic acid, 5-methoxy-3-methylpentyl pentyl ester

Inchi: InChI=1S/C19H36O5/c1-6-9-10-13-23-17(20)19(7-2,8-3)18(21)24-15-12-16(4)11-14-22-5

InchiKey: RPZBXCWZQHQPHY-UHFFFAOYSA-N

Formula: C19H36O5

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCOC

Mol. weight [g/mol]: 344.49

Physical Properties

Property code	Value	Unit	Source
gf	-463.34	kJ/mol	Joback Method
hf	-1071.34	kJ/mol	Joback Method
hfus	40.79	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	4.132		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2027.00		NIST Webbook
rinpol	2027.00		NIST Webbook
tb	805.45	K	Joback Method
tc	992.66	K	Joback Method
tf	457.86	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.83	J/mol×K	805.45	Joback Method
cpg	959.54	J/mol×K	836.65	Joback Method
cpg	976.17	J/mol×K	867.85	Joback Method
cpg	991.75	J/mol×K	899.06	Joback Method
cpg	1006.28	J/mol×K	930.26	Joback Method
cpg	1019.79	J/mol×K	961.46	Joback Method
cpg	1032.30	J/mol×K	992.66	Joback Method
dvisc	0.0007172	Pa×s	457.86	Joback Method

dvisc	0.0003242	Pa×s	515.79	Joback Method
dvisc	0.0001720	Pa×s	573.72	Joback Method
dvisc	0.0001026	Pa×s	631.65	Joback Method
dvisc	0.0000667	Pa×s	689.59	Joback Method
dvisc	0.0000464	Pa×s	747.52	Joback Method
dvisc	0.0000339	Pa×s	805.45	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=U370765&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