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

Inchi: InChI=1S/C20H38O5/c1-6-9-10-11-14-24-18(21)20(7-2,8-3)19(22)25-16-13-17(4)12-15-2
InchiKey: XPXNKBZXKDGXKC-UHFFFAOYSA-N
Formula: C20H38O5
SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCOC
Mol. weight [g/mol]: 358.51

Physical Properties

Property code	Value	Unit	Source
gf	-454.92	kJ/mol	Joback Method
hf	-1091.98	kJ/mol	Joback Method
hfus	43.38	kJ/mol	Joback Method
hvap	79.15	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.522		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1084.92	kPa	Joback Method
rinpol	2117.00		NIST Webbook
tb	828.33	K	Joback Method
tc	1017.82	K	Joback Method
tf	469.13	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.14	J/mol×K	828.33	Joback Method
cpg	1020.16	J/mol×K	859.91	Joback Method
cpg	1037.05	J/mol×K	891.49	Joback Method
cpg	1052.82	J/mol×K	923.08	Joback Method
cpg	1067.49	J/mol×K	954.66	Joback Method
cpg	1081.09	J/mol×K	986.24	Joback Method
cpg	1093.65	J/mol×K	1017.82	Joback Method
dvisc	0.0006309	Pa×s	469.13	Joback Method
dvisc	0.0002825	Pa×s	529.00	Joback Method

dvisc	0.0001489	Pa×s	588.86	Joback Method
dvisc	0.0000884	Pa×s	648.73	Joback Method
dvisc	0.0000573	Pa×s	708.60	Joback Method
dvisc	0.0000397	Pa×s	768.46	Joback Method
dvisc	0.0000290	Pa×s	828.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370766&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

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