Diethylmalonic acid, di(2-octyl) ester

Inchi: InChI=1S/C23H44O4/c1-7-11-13-15-17-19(5)26-21(24)23(9-3,10-4)22(25)27-20(6)18-16-
InchiKey: SSWHDFOWSMCOKF-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CCCCCCC(C)OC(=O)C(CC)(CC)C(=O)OC(C)CCCCCC
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-327.10	kJ/mol	Joback Method
hf	-1026.96	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.597		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	918.83	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	874.11	K	Joback Method
tc	1070.79	K	Joback Method
tf	465.71	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.68	J/mol×K	874.11	Joback Method
cpg	1175.09	J/mol×K	906.89	Joback Method
cpg	1193.24	J/mol×K	939.67	Joback Method
cpg	1210.18	J/mol×K	972.45	Joback Method
cpg	1225.94	J/mol×K	1005.23	Joback Method
cpg	1240.57	J/mol×K	1038.01	Joback Method
cpg	1254.12	J/mol×K	1070.79	Joback Method
dvisc	0.0007729	Pa×s	465.71	Joback Method

dvisc	0.0002941	Pa×s	533.78	Joback Method
dvisc	0.0001392	Pa×s	601.84	Joback Method
dvisc	0.0000767	Pa×s	669.91	Joback Method
dvisc	0.0000472	Pa×s	737.98	Joback Method
dvisc	0.0000315	Pa×s	806.04	Joback Method
dvisc	0.0000224	Pa×s	874.11	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=U369379&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

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