Malonic acid, hexadecyl isobutyl ester

Inchi: InChI=1S/C23H44O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-26-22(24)19-23(25)27
InchiKey: NVKNMHHJNRCDBI-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CC(=O)OCC(C)C
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-327.50	kJ/mol	Joback Method
hf	-1012.93	kJ/mol	Joback Method
hfus	57.38	kJ/mol	Joback Method
hvap	84.72	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.600		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinpol	2581.00		NIST Webbook
tb	877.78	K	Joback Method
tc	1074.72	K	Joback Method
tf	478.29	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.96	J/mol×K	877.78	Joback Method
cpg	1174.58	J/mol×K	910.60	Joback Method
cpg	1192.90	J/mol×K	943.43	Joback Method
cpg	1209.94	J/mol×K	976.25	Joback Method
cpg	1225.74	J/mol×K	1009.07	Joback Method
cpg	1240.32	J/mol×K	1041.89	Joback Method
cpg	1253.72	J/mol×K	1074.72	Joback Method
dvisc	0.0006901	Pa×s	478.29	Joback Method
dvisc	0.0003008	Pa×s	544.87	Joback Method

dvisc	0.0001571	Pa×s	611.45	Joback Method
dvisc	0.0000932	Pa×s	678.03	Joback Method
dvisc	0.0000607	Pa×s	744.62	Joback Method
dvisc	0.0000424	Pa×s	811.20	Joback Method
dvisc	0.0000313	Pa×s	877.78	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=U349112&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

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