Malonic acid, dodecyl 3-methylpentyl ester

Inchi: InChI=1S/C21H40O4/c1-4-6-7-8-9-10-11-12-13-14-16-24-20(22)18-21(23)25-17-15-19(3
InchiKey: NVNBWIXPCLODIW-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCCCCCCCCCCOC(=O)CC(=O)OCCC(C)CC
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-344.34	kJ/mol	Joback Method
hf	-971.65	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Joback Method
hvap	80.26	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.820		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook
tb	832.02	K	Joback Method
tc	1019.80	K	Joback Method
tf	455.75	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.73	J/mol×K	832.02	Joback Method
cpg	1049.46	J/mol×K	863.32	Joback Method
cpg	1067.07	J/mol×K	894.61	Joback Method
cpg	1083.56	J/mol×K	925.91	Joback Method
cpg	1098.97	J/mol×K	957.21	Joback Method
cpg	1113.31	J/mol×K	988.51	Joback Method
cpg	1126.61	J/mol×K	1019.80	Joback Method
dvisc	0.0008818	Pa×s	455.75	Joback Method

dvisc	0.0003912	Pa×s	518.46	Joback Method
dvisc	0.0002068	Pa×s	581.17	Joback Method
dvisc	0.0001238	Pa×s	643.88	Joback Method
dvisc	0.0000812	Pa×s	706.60	Joback Method
dvisc	0.0000570	Pa×s	769.31	Joback Method
dvisc	0.0000422	Pa×s	832.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348286&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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