Malonic acid, 3-methylpentyl pentyl ester

Inchi: InChI=1S/C14H26O4/c1-4-6-7-9-17-13(15)11-14(16)18-10-8-12(3)5-2/h12H,4-11H2,1-3H
InchiKey: RHFUPFGBAMJTED-UHFFFAOYSA-N
Formula: C14H26O4
SMILES: CCCCCOC(=O)CC(=O)OCCC(C)CC
Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
gf	-403.28	kJ/mol	Joback Method
hf	-827.17	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.089		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	1699.00		NIST Webbook
tb	671.86	K	Joback Method
tc	850.20	K	Joback Method
tf	376.86	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.64	J/mol×K	671.86	Joback Method
cpg	638.53	J/mol×K	701.58	Joback Method
cpg	653.66	J/mol×K	731.31	Joback Method
cpg	668.05	J/mol×K	761.03	Joback Method
cpg	681.70	J/mol×K	790.75	Joback Method
cpg	694.61	J/mol×K	820.48	Joback Method
cpg	706.79	J/mol×K	850.20	Joback Method
dvisc	0.0018269	Pa×s	376.86	Joback Method
dvisc	0.0008752	Pa×s	426.03	Joback Method

dvisc	0.0004883	Pa×s	475.19	Joback Method
dvisc	0.0003039	Pa×s	524.36	Joback Method
dvisc	0.0002052	Pa×s	573.53	Joback Method
dvisc	0.0001474	Pa×s	622.69	Joback Method
dvisc	0.0001111	Pa×s	671.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348674&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

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