Malonic acid, 3-heptyl isobutyl ester

Inchi: InChI=1S/C14H26O4/c1-5-7-8-12(6-2)18-14(16)9-13(15)17-10-11(3)4/h11-12H,5-10H2,1
InchiKey: QWBOHEDQDBEVCB-UHFFFAOYSA-N
Formula: C14H26O4
SMILES: CCCCC(CC)OC(=O)CC(=O)OCC(C)C
Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
gf	-405.72	kJ/mol	Joback Method
hf	-832.45	kJ/mol	Joback Method
hfus	30.54	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.088		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	1579.00		NIST Webbook
tb	671.42	K	Joback Method
tc	852.27	K	Joback Method
tf	361.86	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.10	J/mol×K	671.42	Joback Method
cpg	639.24	J/mol×K	701.56	Joback Method
cpg	654.60	J/mol×K	731.70	Joback Method
cpg	669.19	J/mol×K	761.84	Joback Method
cpg	683.00	J/mol×K	791.99	Joback Method
cpg	696.05	J/mol×K	822.13	Joback Method
cpg	708.34	J/mol×K	852.27	Joback Method
dvisc	0.0023105	Pa×s	361.86	Joback Method
dvisc	0.0009958	Pa×s	413.45	Joback Method

dvisc	0.0005173	Pa×s	465.05	Joback Method
dvisc	0.0003062	Pa×s	516.64	Joback Method
dvisc	0.0001994	Pa×s	568.23	Joback Method
dvisc	0.0001395	Pa×s	619.83	Joback Method
dvisc	0.0001031	Pa×s	671.42	Joback Method

Sources

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=U349148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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