

Malonic acid, isohexyl 3-methylbutyl ester

Inchi:	InChI=1S/C14H26O4/c1-11(2)6-5-8-17-13(15)10-14(16)18-9-7-12(3)4/h11-12H,5-10H2,1
InchiKey:	DBYOCVXHFVRQRG-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	CC(C)CCCOC(=O)CC(=O)OCCC(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	-2.92		Crippen Method
logp	2.945		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	1644.00		NIST Webbook
rinpol	1644.00		NIST Webbook
tb	671.42	K	Joback Method
tc	852.27	K	Joback Method
tf	361.86	K	Joback Method
vc	0.856	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.10	J/molxK	671.42	Joback Method
cpg	696.05	J/molxK	822.13	Joback Method
cpg	683.00	J/molxK	791.99	Joback Method
cpg	669.19	J/molxK	761.84	Joback Method
cpg	654.60	J/molxK	731.70	Joback Method
cpg	639.24	J/molxK	701.56	Joback Method
cpg	708.34	J/molxK	852.27	Joback Method
dvisc	0.0001031	Paxs	671.42	Joback Method

dvisc	0.0001395	Paxs	619.83	Joback Method
dvisc	0.0001994	Paxs	568.23	Joback Method
dvisc	0.0003062	Paxs	516.64	Joback Method
dvisc	0.0005173	Paxs	465.05	Joback Method
dvisc	0.0009958	Paxs	413.45	Joback Method
dvisc	0.0023105	Paxs	361.86	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=U348980&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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