

Malonic acid, 2-hexyl isobutyl ester

Inchi:	InChI=1S/C13H24O4/c1-5-6-7-11(4)17-13(15)8-12(14)16-9-10(2)3/h10-11H,5-9H2,1-4H3
InchiKey:	XVAPTGDDNBTBIR-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	CCCCC(C)OC(=O)CC(=O)OCC(C)C
Mol. weight [g/mol]:	244.33

Physical Properties

Property code	Value	Unit	Source
gf	-414.14	kJ/mol	Joback Method
hf	-811.81	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.698		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1519.00		NIST Webbook
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tb	648.54	K	Joback Method
tc	830.39	K	Joback Method
tf	350.59	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.26	J/molxK	648.54	Joback Method
cpg	584.92	J/molxK	678.85	Joback Method
cpg	599.84	J/molxK	709.16	Joback Method
cpg	614.03	J/molxK	739.46	Joback Method
cpg	627.48	J/molxK	769.77	Joback Method
cpg	640.21	J/molxK	800.08	Joback Method
cpg	652.22	J/molxK	830.39	Joback Method
dvisc	0.0025317	Paxs	350.59	Joback Method

dvisc	0.0011034	Paxs	400.25	Joback Method
dvisc	0.0005777	Paxs	449.91	Joback Method
dvisc	0.0003440	Paxs	499.56	Joback Method
dvisc	0.0002249	Paxs	549.22	Joback Method
dvisc	0.0001578	Paxs	598.88	Joback Method
dvisc	0.0001169	Paxs	648.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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