

Malonic acid, isobutyl pentyl ester

Inchi:	InChI=1S/C12H22O4/c1-4-5-6-7-15-11(13)8-12(14)16-9-10(2)3/h10H,4-9H2,1-3H3
InchiKey:	FIDXGGBKDVUQJ-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CCCCCOC(=O)CC(=O)OCC(C)C
Mol. weight [g/mol]:	230.30

Physical Properties

Property code	Value	Unit	Source
gf	-420.12	kJ/mol	Joback Method
hf	-785.89	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.309		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpola	1498.00		NIST Webbook
tb	626.10	K	Joback Method
tc	806.33	K	Joback Method
tf	354.32	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.38	J/molxK	626.10	Joback Method
cpg	531.21	J/molxK	656.14	Joback Method
cpg	545.37	J/molxK	686.18	Joback Method
cpg	558.88	J/molxK	716.21	Joback Method
cpg	571.72	J/molxK	746.25	Joback Method
cpg	583.91	J/molxK	776.29	Joback Method
cpg	595.44	J/molxK	806.33	Joback Method
dvisc	0.0021379	Paxs	354.32	Joback Method
dvisc	0.0010527	Paxs	399.62	Joback Method

dvisc	0.0005987	Paxs	444.91	Joback Method
dvisc	0.0003780	Paxs	490.21	Joback Method
dvisc	0.0002579	Paxs	535.51	Joback Method
dvisc	0.0001868	Paxs	580.80	Joback Method
dvisc	0.0001418	Paxs	626.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349102&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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