

Malonic acid, 2,4-dimethylpent-3-yl isobutyl ester

Inchi:	InChI=1S/C14H26O4/c1-9(2)8-17-12(15)7-13(16)18-14(10(3)4)11(5)6/h9-11,14H,7-8H2,
InchiKey:	BANWDECBRTURCN-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	CC(C)COC(=O)CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	258.35

Physical Properties

Property code	Value	Unit	Source
gf	-410.60	kJ/mol	Joback Method
hf	-843.01	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	63.52	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.800		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpola	1536.00		NIST Webbook
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tb	670.54	K	Joback Method
tc	856.79	K	Joback Method
tf	331.86	K	Joback Method
vc	0.844	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.02	J/molxK	670.54	Joback Method
cpg	640.70	J/molxK	701.58	Joback Method
cpg	656.54	J/molxK	732.62	Joback Method
cpg	671.54	J/molxK	763.67	Joback Method
cpg	685.72	J/molxK	794.71	Joback Method
cpg	699.06	J/molxK	825.75	Joback Method
cpg	711.58	J/molxK	856.79	Joback Method
dvisc	0.0040844	Paxs	331.86	Joback Method

dvisc	0.0013564	Paxs	388.31	Joback Method
dvisc	0.0005959	Paxs	444.75	Joback Method
dvisc	0.0003151	Paxs	501.20	Joback Method
dvisc	0.0001895	Paxs	557.65	Joback Method
dvisc	0.0001252	Paxs	614.09	Joback Method
dvisc	0.0000887	Paxs	670.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349010&Units=SI

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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