

Malonic acid, isobutyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C13H24O4/c1-9(2)6-11(5)17-13(15)7-12(14)16-8-10(3)4/h9-11H,6-8H2,1-5H3
InchiKey:	JLFCGOHNNGILFF-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	CC(C)COC(=O)CC(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	244.33

Physical Properties

Property code	Value	Unit	Source
gf	-416.58	kJ/mol	Joback Method
hf	-817.09	kJ/mol	Joback Method
hfus	24.43	kJ/mol	Joback Method
hvap	61.68	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.554		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpola	1469.00		NIST Webbook
tb	648.10	K	Joback Method
tc	832.83	K	Joback Method
tf	335.59	K	Joback Method
vc	0.793	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.70	J/molxK	648.10	Joback Method
cpg	641.76	J/molxK	802.04	Joback Method
cpg	628.87	J/molxK	771.25	Joback Method
cpg	615.23	J/molxK	740.46	Joback Method
cpg	600.82	J/molxK	709.68	Joback Method
cpg	585.64	J/molxK	678.89	Joback Method
cpg	653.89	J/molxK	832.83	Joback Method
dvisc	0.0001087	Paxs	648.10	Joback Method
dvisc	0.0001499	Paxs	596.02	Joback Method

dvisc	0.0002198	Paxs	543.93	Joback Method
dvisc	0.0003497	Paxs	491.85	Joback Method
dvisc	0.0006210	Paxs	439.76	Joback Method
dvisc	0.0012868	Paxs	387.68	Joback Method
dvisc	0.0033428	Paxs	335.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349332&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

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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