

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

Inchi:	InChI=1S/C14H26O4/c1-6-7-8-17-12(15)9-13(16)18-14(10(2)3)11(4)5/h10-11,14H,6-9H2
InchiKey:	JKYAHRAOWGZXLL-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	CCCCOC(=O)CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	258.35

Physical Properties

Property code	Value	Unit	Source
gf	-408.16	kJ/mol	Joback Method
hf	-837.73	kJ/mol	Joback Method
hfus	27.02	kJ/mol	Joback Method
hvap	63.91	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.944		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpola	1576.00		NIST Webbook
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tb	670.98	K	Joback Method
tc	854.46	K	Joback Method
tf	346.86	K	Joback Method
vc	0.850	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.56	J/molxK	670.98	Joback Method
cpg	697.54	J/molxK	823.88	Joback Method
cpg	684.34	J/molxK	793.30	Joback Method
cpg	670.35	J/molxK	762.72	Joback Method
cpg	655.56	J/molxK	732.14	Joback Method
cpg	639.97	J/molxK	701.56	Joback Method
cpg	709.94	J/molxK	854.46	Joback Method
dvisc	0.0000956	Paxs	670.98	Joback Method

dvisc	0.0001321	Paxs	616.96	Joback Method
dvisc	0.0001942	Paxs	562.94	Joback Method
dvisc	0.0003099	Paxs	508.92	Joback Method
dvisc	0.0005527	Paxs	454.90	Joback Method
dvisc	0.0011517	Paxs	400.88	Joback Method
dvisc	0.0030168	Paxs	346.86	Joback Method

Sources

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=U349011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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