

Malonic acid, di(2-methylpent-3-yl) ester

Inchi:	InChI=1S/C15H28O4/c1-7-12(10(3)4)18-14(16)9-15(17)19-13(8-2)11(5)6/h10-13H,7-9H2
InchiKey:	UBMWNODVATVFNV-UHFFFAOYSA-N
Formula:	C15H28O4
SMILES:	CCC(OC(=O)CC(=O)OC(CC)C(C)C)C(C)C
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
gf	-402.18	kJ/mol	Joback Method
hf	-863.65	kJ/mol	Joback Method
hfus	26.09	kJ/mol	Joback Method
hvap	65.74	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.332		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinqol	1608.00		NIST Webbook
tb	693.42	K	Joback Method
tc	878.58	K	Joback Method
tf	343.13	K	Joback Method
vc	0.899	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.17	J/molxK	693.42	Joback Method
cpg	696.25	J/molxK	724.28	Joback Method
cpg	712.44	J/molxK	755.14	Joback Method
cpg	727.76	J/molxK	786.00	Joback Method
cpg	742.20	J/molxK	816.86	Joback Method
cpg	755.78	J/molxK	847.72	Joback Method
cpg	768.51	J/molxK	878.58	Joback Method
dvisc	0.0036197	Paxs	343.13	Joback Method
dvisc	0.0011973	Paxs	401.51	Joback Method

dvisc	0.0005245	Paxs	459.89	Joback Method
dvisc	0.0002767	Paxs	518.27	Joback Method
dvisc	0.0001662	Paxs	576.66	Joback Method
dvisc	0.0001096	Paxs	635.04	Joback Method
dvisc	0.0000775	Paxs	693.42	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=U349057&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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