

Dimethylmalonic acid, butyl cis-4-methylcyclohexyl ester

Inchi:	InChI=1S/C16H28O4/c1-5-6-11-19-14(17)16(3,4)15(18)20-13-9-7-12(2)8-10-13/h12-13H
InchiKey:	IQLMLIBQNRYYIY-UHFFFAOYSA-N
Formula:	C16H28O4
SMILES:	CCCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-364.42	kJ/mol	Joback Method
hf	-837.94	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.478		Crippen Method
mcvol	240.320	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	1853.00		NIST Webbook
tb	729.71	K	Joback Method
tc	934.09	K	Joback Method
tf	419.96	K	Joback Method
vc	0.900	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.32	J/molxK	729.71	Joback Method
cpg	752.62	J/molxK	763.77	Joback Method
cpg	770.65	J/molxK	797.84	Joback Method
cpg	787.44	J/molxK	831.90	Joback Method
cpg	803.02	J/molxK	865.96	Joback Method
cpg	817.41	J/molxK	900.03	Joback Method
cpg	830.64	J/molxK	934.09	Joback Method
dvisc	0.0014733	Paxs	419.96	Joback Method
dvisc	0.0007344	Paxs	471.59	Joback Method

dvisc	0.0004200	Paxs	523.21	Joback Method
dvisc	0.0002656	Paxs	574.84	Joback Method
dvisc	0.0001811	Paxs	626.46	Joback Method
dvisc	0.0001309	Paxs	678.09	Joback Method
dvisc	0.0000991	Paxs	729.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363876&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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