

Dimethylmalonic acid, butyl 4-chlorophenyl ester

Inchi:	InChI=1S/C15H19ClO4/c1-4-5-10-19-13(17)15(2,3)14(18)20-12-8-6-11(16)7-9-12/h6-9H
InchiKey:	NXIMSNQVGOCHGD-UHFFFAOYSA-N
Formula:	C15H19ClO4
SMILES:	CCCCOC(=O)C(C)(C)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	298.76

Physical Properties

Property code	Value	Unit	Source
gf	-298.73	kJ/mol	Joback Method
hf	-641.96	kJ/mol	Joback Method
hfus	30.62	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.615		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	1900.00		NIST Webbook
tb	761.04	K	Joback Method
tc	977.37	K	Joback Method
tf	474.41	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.21	J/molxK	761.04	Joback Method
cpg	636.18	J/molxK	797.09	Joback Method
cpg	649.11	J/molxK	833.15	Joback Method
cpg	661.04	J/molxK	869.20	Joback Method
cpg	671.99	J/molxK	905.26	Joback Method
cpg	682.01	J/molxK	941.31	Joback Method
cpg	691.13	J/molxK	977.37	Joback Method
dvisc	0.0007431	Paxs	474.41	Joback Method
dvisc	0.0004286	Paxs	522.18	Joback Method

dvisc	0.0002711	Paxs	569.95	Joback Method
dvisc	0.0001841	Paxs	617.73	Joback Method
dvisc	0.0001321	Paxs	665.50	Joback Method
dvisc	0.0000992	Paxs	713.27	Joback Method
dvisc	0.0000771	Paxs	761.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361973&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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