Dimethylmalonic acid, butyl phenyl ester

Inchi: InChI=1S/C15H20O4/c1-4-5-11-18-13(16)15(2,3)14(17)19-12-9-7-6-8-10-12/h6-10H,4-5,
InchiKey: WQRWFMDAPOGDQN-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	-277.17	kJ/mol	Joback Method
hf	-614.75	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	68.28	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.961		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	1719.00		NIST Webbook
rinpol	1719.00		NIST Webbook
tb	718.63	K	Joback Method
tc	930.98	K	Joback Method
tf	431.97	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.90	J/mol×K	718.63	Joback Method
cpg	612.22	J/mol×K	754.02	Joback Method
cpg	626.46	J/mol×K	789.41	Joback Method
cpg	639.68	J/mol×K	824.81	Joback Method
cpg	651.90	J/mol×K	860.20	Joback Method
cpg	663.17	J/mol×K	895.59	Joback Method
cpg	673.51	J/mol×K	930.98	Joback Method
dvisc	0.0010981	Pa×s	431.97	Joback Method

dvisc	0.0005847	Pa×s	479.75	Joback Method
dvisc	0.0003490	Pa×s	527.52	Joback Method
dvisc	0.0002270	Pa×s	575.30	Joback Method
dvisc	0.0001577	Pa×s	623.08	Joback Method
dvisc	0.0001154	Pa×s	670.85	Joback Method
dvisc	0.0000880	Pa×s	718.63	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=U361808&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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