Propanedioic acid, dicyclohexyl ester

Other names: Dicyclohexyl malonate
Inchi: InChI=1S/C15H24O4/c16-14(18-12-7-3-1-4-8-12)11-15(17)19-13-9-5-2-6-10-13/h12-13H
InchiKey: XNLLIRWJZUWAAJ-UHFFFAOYSA-N
Formula: C15H24O4
SMILES: O=C(CC(=O)OC1CCCCC1)OC1CCCCC1
Mol. weight [g/mol]: 268.35
CAS: 1152-57-4

Physical Properties

Property code	Value	Unit	Source
gf	-343.52	kJ/mol	Joback Method
hf	-733.89	kJ/mol	Joback Method
hfus	23.85	kJ/mol	Joback Method
hvap	93.70 ± 1.10	kJ/mol	NIST Webbook
log10ws	-3.84		Crippen Method
logp	3.128		Crippen Method
mcvol	215.370	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	734.28	K	Joback Method
tc	960.99	K	Joback Method
tf	417.89	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.95	J/mol×K	734.28	Joback Method
cpg	753.99	J/mol×K	923.20	Joback Method

cpg	739.70	J/mol×K	885.42	Joback Method
cpg	723.86	J/mol×K	847.63	Joback Method
cpg	706.48	J/mol×K	809.85	Joback Method
cpg	687.51	J/mol×K	772.06	Joback Method
cpg	766.76	J/mol×K	960.99	Joback Method
dvisc	0.0001150	Pa×s	734.28	Joback Method
dvisc	0.0001529	Pa×s	681.55	Joback Method
dvisc	0.0002134	Pa×s	628.82	Joback Method
dvisc	0.0003165	Pa×s	576.09	Joback Method
dvisc	0.0005083	Pa×s	523.35	Joback Method
dvisc	0.0009076	Pa×s	470.62	Joback Method
dvisc	0.0018759	Pa×s	417.89	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1152574&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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