Oxalic acid, dicyclohexyl ester

Other names: Dicyclohexyl oxalate
Ethanedioic acid, dicyclohexyl ester
Inchi: InChI=1S/C14H22O4/c15-13(17-11-7-3-1-4-8-11)14(16)18-12-9-5-2-6-10-12/h11-12H,1-
InchiKey: YJZRTAHDRCUJQT-UHFFFAOYSA-N
Formula: C14H22O4
SMILES: O=C(OC1CCCCC1)C(=O)OC1CCCCC1
Mol. weight [g/mol]: 254.32
CAS: 620-82-6

Physical Properties

Property code	Value	Unit	Source
gf	-351.94	kJ/mol	Joback Method
hf	-713.25	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	92.10 ± 0.70	kJ/mol	NIST Webbook
log10ws	-3.42		Crippen Method
logp	2.738		Crippen Method
mcvol	201.280	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1846.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tb	711.40	K	Joback Method
tc	942.18	K	Joback Method
tf	406.62	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	610.29	J/mol×K	711.40	Joback Method
cpg	630.87	J/mol×K	749.86	Joback Method
cpg	649.86	J/mol×K	788.33	Joback Method
cpg	667.29	J/mol×K	826.79	Joback Method
cpg	683.17	J/mol×K	865.26	Joback Method
cpg	697.51	J/mol×K	903.72	Joback Method
cpg	710.34	J/mol×K	942.18	Joback Method
dvisc	0.0020594	Pa×s	406.62	Joback Method
dvisc	0.0010086	Pa×s	457.42	Joback Method
dvisc	0.0005698	Pa×s	508.21	Joback Method
dvisc	0.0003570	Pa×s	559.01	Joback Method
dvisc	0.0002419	Pa×s	609.81	Joback Method
dvisc	0.0001740	Pa×s	660.60	Joback Method
dvisc	0.0001311	Pa×s	711.40	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C620826&Units=SI

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