

1,2-Cyclohexanedicarboxylic acid, 3-chlorophenyl ethyl ester

Inchi: InChI=1S/C16H19ClO4/c1-2-20-15(18)13-8-3-4-9-14(13)16(19)21-12-7-5-6-11(17)10-12
InchiKey: HXTYQKYEEFRHHB-UHFFFAOYSA-N
Formula: C16H19ClO4
SMILES: CCOC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-276.41	kJ/mol	Joback Method
hf	-619.87	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	76.97	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.615		Crippen Method
mvol	228.800	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	802.03	K	Joback Method
tc	1034.41	K	Joback Method
tf	486.40	K	Joback Method
vc	0.853	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.35	J/molxK	802.03	Joback Method
cpg	737.22	J/molxK	995.68	Joback Method
cpg	727.13	J/molxK	956.95	Joback Method
cpg	715.61	J/molxK	918.22	Joback Method
cpg	702.65	J/molxK	879.49	Joback Method
cpg	688.24	J/molxK	840.76	Joback Method
cpg	745.90	J/molxK	1034.41	Joback Method
dvisc	0.0001095	Paxs	802.03	Joback Method

dvisc	0.0001373	Paxs	749.42	Joback Method
dvisc	0.0001781	Paxs	696.82	Joback Method
dvisc	0.0002411	Paxs	644.22	Joback Method
dvisc	0.0003444	Paxs	591.61	Joback Method
dvisc	0.0005274	Paxs	539.00	Joback Method
dvisc	0.0008856	Paxs	486.40	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339690&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

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