

1,2-Cyclohexanedicarboxylic acid, 2,5-dichlorophenyl ethyl ester

Inchi:	InChI=1S/C16H18Cl2O4/c1-2-21-15(19)11-5-3-4-6-12(11)16(20)22-14-9-10(17)7-8-13(14)
InchiKey:	RIAVCMRJFXTERK-UHFFFAOYSA-N
Formula:	C16H18Cl2O4
SMILES:	CCOC(=O)C1CCCCC1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	345.22

Physical Properties

Property code	Value	Unit	Source
gf	-297.97	kJ/mol	Joback Method
hf	-647.08	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	82.01	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.268		Crippen Method
mvol	241.040	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook
tb	844.44	K	Joback Method
tc	1080.07	K	Joback Method
tf	528.84	K	Joback Method
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.04	J/molxK	844.44	Joback Method
cpg	752.14	J/molxK	1040.80	Joback Method
cpg	743.84	J/molxK	1001.53	Joback Method
cpg	734.09	J/molxK	962.26	Joback Method
cpg	722.88	J/molxK	922.98	Joback Method
cpg	710.20	J/molxK	883.71	Joback Method
cpg	758.99	J/molxK	1080.07	Joback Method
dvisc	0.0000977	Paxs	844.44	Joback Method

dvisc	0.0001208	Paxs	791.84	Joback Method
dvisc	0.0001540	Paxs	739.24	Joback Method
dvisc	0.0002038	Paxs	686.64	Joback Method
dvisc	0.0002826	Paxs	634.04	Joback Method
dvisc	0.0004156	Paxs	581.44	Joback Method
dvisc	0.0006600	Paxs	528.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339795&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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