

1,2-Cyclohexanedicarboxylic acid, 2-chloroethyl pentyl ester

Inchi:	InChI=1S/C15H25ClO4/c1-2-3-6-10-19-14(17)12-7-4-5-8-13(12)15(18)20-11-9-16/h12-13
InchiKey:	MYDXJQWVAFPPRE-UHFFFAOYSA-N
Formula:	C15H25ClO4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCCCl
Mol. weight [g/mol]:	304.81

Physical Properties

Property code	Value	Unit	Source
gf	-387.61	kJ/mol	Joback Method
hf	-824.29	kJ/mol	Joback Method
hfus	37.28	kJ/mol	Joback Method
hvap	71.80	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.308		Crippen Method
mvol	238.470	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2063.00		NIST Webbook
tb	747.49	K	Joback Method
tc	948.91	K	Joback Method
tf	436.19	K	Joback Method
vc	0.904	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.56	J/molxK	747.49	Joback Method
cpg	722.91	J/molxK	781.06	Joback Method
cpg	739.11	J/molxK	814.63	Joback Method
cpg	754.17	J/molxK	848.20	Joback Method
cpg	768.10	J/molxK	881.77	Joback Method
cpg	780.90	J/molxK	915.34	Joback Method
cpg	792.59	J/molxK	948.91	Joback Method
dvisc	0.0013293	Paxs	436.19	Joback Method

dvisc	0.0007215	Paxs	488.07	Joback Method
dvisc	0.0004404	Paxs	539.96	Joback Method
dvisc	0.0002931	Paxs	591.84	Joback Method
dvisc	0.0002083	Paxs	643.72	Joback Method
dvisc	0.0001558	Paxs	695.61	Joback Method
dvisc	0.0001213	Paxs	747.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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