

1,2-Cyclohexanedicarboxylic acid, 4-chloro-3-methylphenyl isoheptyl ester

Inchi:	InChI=1S/C21H29ClO4/c1-14(2)7-6-12-25-20(23)17-8-4-5-9-18(17)21(24)26-16-10-11-19
InchiKey:	MWBBLORVHUOWHG-UHFFFAOYSA-N
Formula:	C21H29ClO4
SMILES:	Cc1cc(OC(=O)C2CCCCC2C(=O)OCCCC(C)C)ccc1Cl
Mol. weight [g/mol]:	380.91

Physical Properties

Property code	Value	Unit	Source
gf	-246.38	kJ/mol	Joback Method
hf	-739.82	kJ/mol	Joback Method
hfus	42.56	kJ/mol	Joback Method
hvap	88.37	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.340		Crippen Method
mvol	299.250	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	2672.00		NIST Webbook
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tb	920.97	K	Joback Method
tc	1146.11	K	Joback Method
tf	540.27	K	Joback Method
vc	1.127	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.76	J/molxK	920.97	Joback Method
cpg	978.37	J/molxK	958.49	Joback Method
cpg	992.33	J/molxK	996.02	Joback Method
cpg	1004.66	J/molxK	1033.54	Joback Method
cpg	1015.40	J/molxK	1071.07	Joback Method
cpg	1024.56	J/molxK	1108.59	Joback Method
cpg	1032.17	J/molxK	1146.11	Joback Method
dvisc	0.0005294	Paxs	540.27	Joback Method

dvisc	0.0002930	Paxs	603.72	Joback Method
dvisc	0.0001815	Paxs	667.17	Joback Method
dvisc	0.0001222	Paxs	730.62	Joback Method
dvisc	0.0000876	Paxs	794.07	Joback Method
dvisc	0.0000660	Paxs	857.52	Joback Method
dvisc	0.0000517	Paxs	920.97	Joback Method

Sources

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=U339688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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