

6-Chlorohexanoic acid, 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C12H12Cl4O2/c13-5-3-1-2-4-12(17)18-11-7-9(15)8(14)6-10(11)16/h6-7H,1-5H
InchiKey:	RWCBWJQSBGXTNB-UHFFFAOYSA-N
Formula:	C12H12Cl4O2
SMILES:	O=C(CCCCCCl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	330.03

Physical Properties

Property code	Value	Unit	Source
gf	-147.96	kJ/mol	Joback Method
hf	-396.65	kJ/mol	Joback Method
hfus	39.28	kJ/mol	Joback Method
hvap	73.26	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	5.351		Crippen Method
mcvol	212.580	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpola	2298.00		NIST Webbook
rinpola	2298.00		NIST Webbook
tb	741.59	K	Joback Method
tc	963.78	K	Joback Method
tf	480.82	K	Joback Method
vc	0.820	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.51	J/molxK	741.59	Joback Method
cpg	502.33	J/molxK	778.62	Joback Method
cpg	512.37	J/molxK	815.65	Joback Method
cpg	521.66	J/molxK	852.69	Joback Method
cpg	530.19	J/molxK	889.72	Joback Method
cpg	538.01	J/molxK	926.75	Joback Method
cpg	545.10	J/molxK	963.78	Joback Method
dvisc	0.0007397	Paxs	480.82	Joback Method

dvisc	0.0004913	Paxs	524.28	Joback Method
dvisc	0.0003474	Paxs	567.74	Joback Method
dvisc	0.0002580	Paxs	611.21	Joback Method
dvisc	0.0001994	Paxs	654.67	Joback Method
dvisc	0.0001591	Paxs	698.13	Joback Method
dvisc	0.0001304	Paxs	741.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354731&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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