

Cyclohexanecarboxylic acid, 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C13H13Cl3O2/c14-9-6-11(16)12(7-10(9)15)18-13(17)8-4-2-1-3-5-8/h6-8H,1-5H
InchiKey:	OQAHIIINXZJWKED-UHFFFAOYSA-N
Formula:	C13H13Cl3O2
SMILES:	O=C(Oc1cc(Cl)c(Cl)cc1Cl)C1CCCCC1
Mol. weight [g/mol]:	307.60

Physical Properties

Property code	Value	Unit	Source
gf	-103.16	kJ/mol	Joback Method
hf	-347.23	kJ/mol	Joback Method
hfus	29.51	kJ/mol	Joback Method
hvap	71.53	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.133		Crippen Method
mcvol	203.570	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	2169.00		NIST Webbook
tb	746.59	K	Joback Method
tc	996.78	K	Joback Method
tf	469.55	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.72	J/molxK	746.59	Joback Method
cpg	526.06	J/molxK	788.29	Joback Method
cpg	539.12	J/molxK	829.99	Joback Method
cpg	550.94	J/molxK	871.69	Joback Method
cpg	561.53	J/molxK	913.39	Joback Method
cpg	570.94	J/molxK	955.09	Joback Method
cpg	579.18	J/molxK	996.78	Joback Method
dvisc	0.0009202	Paxs	469.55	Joback Method
dvisc	0.0005800	Paxs	515.72	Joback Method

dvisc	0.0003944	Paxs	561.90	Joback Method
dvisc	0.0002844	Paxs	608.07	Joback Method
dvisc	0.0002147	Paxs	654.24	Joback Method
dvisc	0.0001682	Paxs	700.42	Joback Method
dvisc	0.0001359	Paxs	746.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354653&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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