

2,4-Ditert-butyl-6-chlorophenyl trichloroacetate

Inchi:	InChI=1S/C16H20Cl4O2/c1-14(2,3)9-7-10(15(4,5)6)12(11(17)8-9)22-13(21)16(18,19)20/
InchiKey:	ZNVSRLBLEMSVUKT-UHFFFAOYSA-N
Formula:	C16H20Cl4O2
SMILES:	CC(C)(C)c1cc(Cl)c(OC(=O)C(Cl)(Cl)Cl)c(C(C)(C)C)c1
Mol. weight [g/mol]:	386.14
CAS:	116436-41-0

Physical Properties

Property code	Value	Unit	Source
gf	-105.76	kJ/mol	Joback Method
hf	-505.46	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	6.211		Crippen Method
mcvol	268.940	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
tb	823.42	K	Joback Method
tc	1064.14	K	Joback Method
tf	533.16	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.10	J/molxK	823.42	Joback Method
cpg	724.28	J/molxK	863.54	Joback Method
cpg	736.43	J/molxK	903.66	Joback Method
cpg	747.68	J/molxK	943.78	Joback Method
cpg	758.14	J/molxK	983.90	Joback Method
cpg	767.93	J/molxK	1024.02	Joback Method
cpg	777.19	J/molxK	1064.14	Joback Method
dvisc	0.0003801	Paxs	533.16	Joback Method
dvisc	0.0002211	Paxs	581.54	Joback Method

dvisc	0.0001398	Paxs	629.91	Joback Method
dvisc	0.0000944	Paxs	678.29	Joback Method
dvisc	0.0000671	Paxs	726.67	Joback Method
dvisc	0.0000498	Paxs	775.04	Joback Method
dvisc	0.0000383	Paxs	823.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116436410&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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