

Tridiphane

Other names:	(.+/-)-2-(3,5-Dichlorophenyl)-2-(2,2,2-trichloroethyl)oxirane (Rs)-2-(3,5-dichlorophenyl)-2-(2,2,2-trichloroethyl)oxirane Dowco 356 Nelpon Tandem 2-(3,5-Dichlorophenyl)-2-(2,2,2-trichloroethyl)oxirane
Inchi:	InChI=1S/C10H7Cl5O/c11-7-1-6(2-8(12)3-7)9(5-16-9)4-10(13,14)15/h1-3H,4-5H2
InchiKey:	IBZH0AONZVJLOB-UHFFFAOYSA-N
Formula:	C10H7Cl5O
SMILES:	Clc1cc(Cl)cc(C2(CC(Cl)(Cl)Cl)CO2)c1
Mol. weight [g/mol]:	320.43
CAS:	58138-08-2

Physical Properties

Property code	Value	Unit	Source
gf	38.80	kJ/mol	Joback Method
hf	-167.55	kJ/mol	Joback Method
hfus	28.31	kJ/mol	Joback Method
hvap	65.35	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.979		Crippen Method
mcvol	184.210	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
tb	682.69	K	Joback Method
tc	949.63	K	Joback Method
tf	315.21 ± 0.20	K	NIST Webbook
vc	0.698	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.67	J/mol×K	905.14	Joback Method
cpg	391.87	J/mol×K	682.69	Joback Method
cpg	401.56	J/mol×K	727.18	Joback Method

cpg	410.67	J/mol×K	771.67	Joback Method
cpg	419.52	J/mol×K	816.16	Joback Method
cpg	428.42	J/mol×K	860.65	Joback Method
cpg	447.60	J/mol×K	949.63	Joback Method
hfust	18.54	kJ/mol	313.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58138082&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/22-446-2/Tridiphane.pdf>

Generated by Cheméo on 2024-05-03 20:35:54.874983707 +0000 UTC m=+17057803.795561070.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.