

2,4,5-Trichlorophenyl diethylthionocarbamate

Inchi:	InChI=1S/C11H12Cl3NOS/c1-3-15(4-2)11(17)16-10-6-8(13)7(12)5-9(10)14/h5-6H,3-4H2
InchiKey:	QQBXAKQJAJFIJG-UHFFFAOYSA-N
Formula:	C11H12Cl3NOS
SMILES:	CCN(CC)C(=S)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	312.64
CAS:	22764-81-4

Physical Properties

Property code	Value	Unit	Source
gf	212.31	kJ/mol	Joback Method
hf	-33.66	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	68.68	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.652		Crippen Method
mcvol	206.710	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
tb	709.89	K	Joback Method
tc	943.70	K	Joback Method
tf	456.44	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.05	J/molxK	709.89	Joback Method
cpg	479.26	J/molxK	748.86	Joback Method
cpg	489.67	J/molxK	787.83	Joback Method
cpg	499.36	J/molxK	826.80	Joback Method
cpg	508.40	J/molxK	865.76	Joback Method
cpg	516.84	J/molxK	904.73	Joback Method
cpg	524.77	J/molxK	943.70	Joback Method

Sources

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=C22764814&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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