3-Trifluoromethylbenzoic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C10H6Cl3F3O2/c11-9(12,13)5-18-8(17)6-2-1-3-7(4-6)10(14,15)16/h1-4H,5H2
InchiKey: JCHPKZAJAAOACB-UHFFFAOYSA-N
Formula: C10H6Cl3F3O2
SMILES: O=C(OCC(Cl)(Cl)Cl)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 321.51

Physical Properties

Property code	Value	Unit	Source
gf	-712.36	kJ/mol	Joback Method
hf	-922.52	kJ/mol	Joback Method
hfus	25.10	kJ/mol	Joback Method
hvap	58.06	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.232		Crippen Method
mcvol	177.470	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1539.00		NIST Webbook
tb	639.79	K	Joback Method
tc	859.54	K	Joback Method
tf	409.93	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.85	J/mol×K	639.79	Joback Method
cpg	414.70	J/mol×K	676.42	Joback Method
cpg	423.64	J/mol×K	713.04	Joback Method
cpg	431.75	J/mol×K	749.67	Joback Method
cpg	439.09	J/mol×K	786.29	Joback Method
cpg	445.73	J/mol×K	822.92	Joback Method
cpg	451.74	J/mol×K	859.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355141&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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