

Tetraethylene glycol, chlorodifluoroacetate, trifluoroacetate

Inchi:	InChI=1S/C12H16ClF5O7/c13-11(14,15)9(19)24-7-5-22-3-1-21-2-4-23-6-8-25-10(20)12(
InchiKey:	LJPZAKYOGARGSN-UHFFFAOYSA-N
Formula:	C12H16ClF5O7
SMILES:	O=C(OCCOCCOCCOCCOC(=O)C(F)(F)Cl)C(F)(F)F
Mol. weight [g/mol]:	402.70

Physical Properties

Property code	Value	Unit	Source
gf	-1712.98	kJ/mol	Joback Method
hf	-2191.06	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	65.56	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.516		Crippen Method
mvol	233.520	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	721.12	K	Joback Method
tc	892.08	K	Joback Method
tf	473.72	K	Joback Method
vc	0.926	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.70	J/molxK	721.12	Joback Method
cpg	682.45	J/molxK	749.61	Joback Method
cpg	693.49	J/molxK	778.11	Joback Method
cpg	703.83	J/molxK	806.60	Joback Method
cpg	713.46	J/molxK	835.09	Joback Method
cpg	722.39	J/molxK	863.58	Joback Method
cpg	730.62	J/molxK	892.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375920&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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