

Tetraethylene glycol, bis(chlorodifluoroacetate)

Inchi: InChI=1S/C12H16Cl2F4O7/c13-11(15,16)9(19)24-7-5-22-3-1-21-2-4-23-6-8-25-10(20)12

InchiKey: UQQGMIVTKDQOOM-UHFFFAOYSA-N

Formula: C12H16Cl2F4O7

SMILES: O=C(OCCOCCOCCOCCOC(=O)C(F)(F)Cl)C(F)(F)Cl

Mol. weight [g/mol]: 419.15

Physical Properties

Property code	Value	Unit	Source
gf	-1530.10	kJ/mol	Joback Method
hf	-2010.69	kJ/mol	Joback Method
hfus	41.86	kJ/mol	Joback Method
hvap	70.76	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.786		Crippen Method
mcvol	243.990	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	1819.00		NIST Webbook
tb	759.28	K	Joback Method
tc	939.41	K	Joback Method
tf	503.05	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.46	J/mol×K	759.28	Joback Method
cpg	699.67	J/mol×K	789.30	Joback Method
cpg	710.10	J/mol×K	819.32	Joback Method
cpg	719.76	J/mol×K	849.35	Joback Method
cpg	728.66	J/mol×K	879.37	Joback Method
cpg	736.78	J/mol×K	909.39	Joback Method
cpg	744.15	J/mol×K	939.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U375919&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
hvac:	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

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