Triethylene glycol, chlorodifluoroacetate, heptafluorobutyrate

Inchi: InChI=1S/C12H12ClF9O6/c13-10(16,17)8(24)28-6-4-26-2-1-25-3-5-27-7(23)9(14,15)11(1

InchiKey: ZDEGNFIPCXNMPL-UHFFFAOYSA-N

Formula: C12H12ClF9O6

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

Mol. weight [g/mol]: 458.66

Physical Properties

Property code	Value	Unit	Source
gf	-2381.54	kJ/mol	Joback Method
hf	-2860.78	kJ/mol	Joback Method
hfus	37.05	kJ/mol	Joback Method
hvap	57.29	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.771		Crippen Method
mcvol	234.730	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
tb	689.32	K	Joback Method
tc	852.13	K	Joback Method
tf	458.69	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.41	J/mol×K	689.32	Joback Method
cpg	692.24	J/mol×K	716.45	Joback Method
cpg	702.36	J/mol×K	743.59	Joback Method
cpg	711.79	J/mol×K	770.72	Joback Method
cpg	720.57	J/mol×K	797.86	Joback Method
cpg	728.73	J/mol×K	824.99	Joback Method
cpg	736.29	J/mol×K	852.13	Joback Method

Sources

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=U375928&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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