2-Pentoxyethyl trifluoroacetate

Inchi: InChI=1S/C9H15F3O3/c1-2-3-4-5-14-6-7-15-8(13)9(10,11)12/h2-7H2,1H3
InchiKey: JFZUZMNTOZLYQH-UHFFFAOYSA-N
Formula: C9H15F3O3
SMILES: CCCCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 228.21

Physical Properties

Property code	Value	Unit	Source
gf	-895.61	kJ/mol	Joback Method
hf	-1203.19	kJ/mol	Joback Method
hfus	24.87	kJ/mol	Joback Method
hvap	43.45	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.299		Crippen Method
mcvol	156.290	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1051.40		NIST Webbook
tb	498.61	K	Joback Method
tc	658.18	K	Joback Method
tf	289.77	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.74	J/mol×K	498.61	Joback Method
cpg	388.00	J/mol×K	525.20	Joback Method
cpg	399.77	J/mol×K	551.80	Joback Method
cpg	411.06	J/mol×K	578.39	Joback Method
cpg	421.88	J/mol×K	604.99	Joback Method
cpg	432.25	J/mol×K	631.58	Joback Method
cpg	442.15	J/mol×K	658.18	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=R188928&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