2-Butoxyethyl 2,2,3,3,3-pentafluoropropanoate

Other names: 2-Butoxyethanol, pentafluoropropionate
Inchi: InChI=1S/C9H13F5O3/c1-2-3-4-16-5-6-17-7(15)8(10,11)9(12,13)14/h2-6H2,1H3
InchiKey: VTVWSBYCVXXAHJ-UHFFFAOYSA-N
Formula: C9H13F5O3
SMILES: CCCCOCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 264.19

Physical Properties

Property code	Value	Unit	Source
gf	-1282.39	kJ/mol	Joback Method
hf	-1604.16	kJ/mol	Joback Method
hfus	23.61	kJ/mol	Joback Method
hvap	40.52	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.544		Crippen Method
mcvol	159.830	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	970.40		NIST Webbook
rinpol	970.40		NIST Webbook
tb	493.92	K	Joback Method
tc	647.91	K	Joback Method
tf	293.37	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.13	J/mol×K	493.92	Joback Method
cpg	407.20	J/mol×K	519.58	Joback Method
cpg	418.73	J/mol×K	545.25	Joback Method
cpg	429.71	J/mol×K	570.91	Joback Method
cpg	440.18	J/mol×K	596.58	Joback Method
cpg	450.13	J/mol×K	622.24	Joback Method
cpg	459.60	J/mol×K	647.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351986&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

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