2-Butoxyethyl 2,2,3,3,4,4,4-heptafluorobutanoate

Other names: 2-Butoxyethanol, heptafluorobutyrate

Inchi: InChI=1S/C10H13F7O3/c1-2-3-4-19-5-6-20-7(18)8(11,12)9(13,14)10(15,16)17/h2-6H2,1

InchiKey: MLLJQNXYWLQZNV-UHFFFAOYSA-N

Formula: C10H13F7O3

SMILES: CCCCOCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 314.20

Physical Properties

Property code	Value	Unit	Source
gf	-1660.75	kJ/mol	Joback Method
hf	-2025.77	kJ/mol	Joback Method
hfus	24.95	kJ/mol	Joback Method
hvap	39.81	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.179		Crippen Method
mcvol	177.460	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1007.60		NIST Webbook
tb	512.11	K	Joback Method
tc	660.80	K	Joback Method
tf	308.24	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.54	J/mol×K	512.11	Joback Method
cpg	473.09	J/mol×K	536.89	Joback Method
cpg	485.01	J/mol×K	561.67	Joback Method
cpg	496.32	J/mol×K	586.45	Joback Method
cpg	507.04	J/mol×K	611.24	Joback Method
cpg	517.19	J/mol×K	636.02	Joback Method
cpg	526.79	J/mol×K	660.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352018&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