1-Butoxypropan-2-yl 2,2,3,3,3-pentafluoropropanoate

Inchi: InChI=1S/C10H15F5O3/c1-3-4-5-17-6-7(2)18-8(16)9(11,12)10(13,14)15/h7H,3-6H2,1-2H

InchiKey: JESFKTHDIYRXMD-UHFFFAOYSA-N

Formula: C10H15F5O3

SMILES: CCCCOCC(C)OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 278.22

Physical Properties

Property code	Value	Unit	Source
gf	-1276.41	kJ/mol	Joback Method
hf	-1630.08	kJ/mol	Joback Method
hfus	22.68	kJ/mol	Joback Method
hvap	42.36	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.932		Crippen Method
mcvol	173.920	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	994.00		NIST Webbook
rinpol	994.00		NIST Webbook
tb	516.36	K	Joback Method
tc	672.68	K	Joback Method
tf	289.64	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.45	J/mol×K	516.36	Joback Method
cpg	454.50	J/mol×K	542.41	Joback Method
cpg	466.95	J/mol×K	568.47	Joback Method
cpg	478.80	J/mol×K	594.52	Joback Method
cpg	490.08	J/mol×K	620.58	Joback Method
cpg	500.81	J/mol×K	646.63	Joback Method
cpg	510.99	J/mol×K	672.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378329&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