1-Propoxypropan-2-ol, heptafluorobutyrate

Inchi: InChI=1S/C10H13F7O3/c1-3-4-19-5-6(2)20-7(18)8(11,12)9(13,14)10(15,16)17/h6H,3-5H
InchiKey: UNPJZAJHYXSFHS-UHFFFAOYSA-N
Formula: C10H13F7O3
SMILES: CCCOCC(C)OC(=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	-1663.19	kJ/mol	Joback Method
hf	-2031.05	kJ/mol	Joback Method
hfus	21.43	kJ/mol	Joback Method
hvap	39.42	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.178		Crippen Method
mcvol	177.460	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	971.00		NIST Webbook
tb	511.67	K	Joback Method
tc	662.83	K	Joback Method
tf	293.24	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.75	J/mol×K	511.67	Joback Method
cpg	473.58	J/mol×K	536.86	Joback Method
cpg	485.74	J/mol×K	562.06	Joback Method
cpg	497.26	J/mol×K	587.25	Joback Method
cpg	508.18	J/mol×K	612.44	Joback Method
cpg	518.50	J/mol×K	637.64	Joback Method
cpg	528.25	J/mol×K	662.83	Joback Method

Sources

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=U378339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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