(S)-(-)-1,2,4-Butanetriol, 4-heptafluorobutyrate

Inchi: InChI=1S/C8H9F7O4/c9-6(10,7(11,12)8(13,14)15)5(18)19-2-1-4(17)3-16/h4,16-17H,1-3H
InchiKey: YPWNLKMJLQCLLR-UHFFFAOYSA-N
Formula: C8H9F7O4
SMILES: O=C(OCCC(O)CO)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 302.14

Physical Properties

Property code	Value	Unit	Source
gf	-1848.67	kJ/mol	Joback Method
hf	-2162.01	kJ/mol	Joback Method
hfus	23.23	kJ/mol	Joback Method
hvap	65.92	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.106		Crippen Method
mcvol	155.150	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1066.00		NIST Webbook
rinpol	1066.00		NIST Webbook
tb	627.85	K	Joback Method
tc	779.93	K	Joback Method
tf	370.11	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.20	J/mol×K	627.85	Joback Method
cpg	460.27	J/mol×K	653.20	Joback Method
cpg	467.83	J/mol×K	678.54	Joback Method
cpg	474.90	J/mol×K	703.89	Joback Method
cpg	481.52	J/mol×K	729.23	Joback Method
cpg	487.71	J/mol×K	754.58	Joback Method
cpg	493.50	J/mol×K	779.93	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=U374872&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