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

Inchi: InChI=1S/C7H9F5O4/c8-6(9,7(10,11)12)5(15)16-2-1-4(14)3-13/h4,13-14H,1-3H2

InchiKey: UJRHXTYAFYZOBS-UHFFFAOYSA-N

Formula: C7H9F5O4

SMILES: O=C(OCCC(O)CO)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 252.14

Physical Properties

Property code	Value	Unit	Source
gf	-1470.31	kJ/mol	Joback Method
hf	-1740.40	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	66.62	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.470		Crippen Method
mcvol	137.520	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	989.00		NIST Webbook
rinpol	989.00		NIST Webbook
tb	609.66	K	Joback Method
tc	764.08	K	Joback Method
tf	355.24	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.02	J/mol×K	609.66	Joback Method
cpg	392.77	J/mol×K	635.40	Joback Method
cpg	400.07	J/mol×K	661.13	Joback Method
cpg	406.94	J/mol×K	686.87	Joback Method
cpg	413.41	J/mol×K	712.61	Joback Method
cpg	419.50	J/mol×K	738.34	Joback Method
cpg	425.22	J/mol×K	764.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374870&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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