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

Inchi: InChI=1S/C6H9F3O4/c7-6(8,9)5(12)13-2-1-4(11)3-10/h4,10-11H,1-3H2
InchiKey: PQQXIPGEDLNBKJ-UHFFFAOYSA-N
Formula: C6H9F3O4
SMILES: O=C(OCCC(O)CO)C(F)(F)F
Mol. weight [g/mol]: 202.13

Physical Properties

Property code	Value	Unit	Source
gf	-1091.95	kJ/mol	Joback Method
hf	-1318.79	kJ/mol	Joback Method
hfus	20.56	kJ/mol	Joback Method
hvap	67.33	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	-0.165		Crippen Method
mcvol	119.890	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	950.00		NIST Webbook
rinpol	950.00		NIST Webbook
tb	591.47	K	Joback Method
tc	749.53	K	Joback Method
tf	340.37	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.85	J/mol×K	591.47	Joback Method
cpg	326.18	J/mol×K	617.81	Joback Method
cpg	333.14	J/mol×K	644.16	Joback Method
cpg	339.75	J/mol×K	670.50	Joback Method
cpg	346.01	J/mol×K	696.85	Joback Method
cpg	351.94	J/mol×K	723.19	Joback Method
cpg	357.55	J/mol×K	749.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374868&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