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

Inchi: InChI=1S/C12H8F14O5/c13-7(14,9(17,18)11(21,22)23)5(28)30-2-1-4(3-27)31-6(29)8(15,

InchiKey: NBPSKUASTBFLKL-UHFFFAOYSA-N

Formula: C12H8F14O5

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

Mol. weight [g/mol]: 498.17

Physical Properties

Property code	Value	Unit	Source
gf	-3267.24	kJ/mol	Joback Method
hf	-3736.16	kJ/mol	Joback Method
hfus	31.61	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.490		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	1377.86	kPa	Joback Method
rinpol	1132.00		NIST Webbook
tb	688.68	K	Joback Method
tc	844.07	K	Joback Method
tf	437.92	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.72	J/mol×K	688.68	Joback Method
cpg	714.03	J/mol×K	714.58	Joback Method
cpg	722.61	J/mol×K	740.48	Joback Method
cpg	730.52	J/mol×K	766.38	Joback Method
cpg	737.80	J/mol×K	792.28	Joback Method
cpg	744.53	J/mol×K	818.17	Joback Method
cpg	750.74	J/mol×K	844.07	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=U374873&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