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

Inchi: InChI=1S/C10H8F10O5/c11-7(12,9(15,16)17)5(22)24-2-1-4(3-21)25-6(23)8(13,14)10(18,

InchiKey: SJKPSOOKCDNRPQ-UHFFFAOYSA-N

Formula: C10H8F10O5

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

Mol. weight [g/mol]: 398.15

Physical Properties

Property code	Value	Unit	Source
gf	-2510.52	kJ/mol	Joback Method
hf	-2892.94	kJ/mol	Joback Method
hfus	28.94	kJ/mol	Joback Method
hvap	59.10	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.219		Crippen Method
mcvol	190.210	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	1063.00		NIST Webbook
tb	652.30	K	Joback Method
tc	806.22	K	Joback Method
tf	408.18	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.55	J/mol×K	652.30	Joback Method
cpg	574.54	J/mol×K	677.95	Joback Method
cpg	582.92	J/mol×K	703.61	Joback Method
cpg	590.71	J/mol×K	729.26	Joback Method
cpg	597.96	J/mol×K	754.92	Joback Method
cpg	604.69	J/mol×K	780.57	Joback Method
cpg	610.94	J/mol×K	806.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374871&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

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