1,2-Propanediol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C11H6F14O4/c1-3(29-5(27)7(14,15)9(18,19)11(23,24)25)2-28-4(26)6(12,13)8(
InchiKey: MCZXUJJEJUJKKZ-UHFFFAOYSA-N
Formula: C11H6F14O4
SMILES: CC(COC(=O)C(F)(F)C(F)(F)C(F)(F)F)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 468.14

Physical Properties

Property code	Value	Unit	Source
gf	-3138.84	kJ/mol	Joback Method
hf	-3563.29	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	38.79	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.127		Crippen Method
mcvol	205.510	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	1049.00		NIST Webbook
rinpol	1049.00		NIST Webbook
tb	573.62	K	Joback Method
tc	716.62	K	Joback Method
tf	365.83	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.60	J/mol×K	573.62	Joback Method
cpg	609.55	J/mol×K	597.45	Joback Method
cpg	619.72	J/mol×K	621.29	Joback Method
cpg	629.16	J/mol×K	645.12	Joback Method
cpg	637.90	J/mol×K	668.96	Joback Method
cpg	646.00	J/mol×K	692.79	Joback Method
cpg	653.48	J/mol×K	716.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375545&Units=SI

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