1,3-Propanediol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C11H6F14O4/c12-6(13,8(16,17)10(20,21)22)4(26)28-2-1-3-29-5(27)7(14,15)9(
InchiKey: GHMHMCMIEVQLKF-UHFFFAOYSA-N
Formula: C11H6F14O4
SMILES: O=C(OCCCOC(=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]: 468.14

Physical Properties

Property code	Value	Unit	Source
gf	-3136.40	kJ/mol	Joback Method
hf	-3558.01	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	39.18	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.129		Crippen Method
mcvol	205.510	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	968.00		NIST Webbook
rinpol	968.00		NIST Webbook
tb	574.06	K	Joback Method
tc	715.55	K	Joback Method
tf	380.83	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.25	J/mol×K	574.06	Joback Method
cpg	609.02	J/mol×K	597.64	Joback Method
cpg	619.05	J/mol×K	621.22	Joback Method
cpg	628.36	J/mol×K	644.81	Joback Method
cpg	637.01	J/mol×K	668.39	Joback Method
cpg	645.01	J/mol×K	691.97	Joback Method
cpg	652.43	J/mol×K	715.55	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=U375556&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