Ethanolamine, N,O-bis(heptafluorobutyryl)-

Inchi: InChI=1S/C10H5F14NO3/c11-5(12,7(15,16)9(19,20)21)3(26)25-1-2-28-4(27)6(13,14)8(1
InchiKey: WESDPPGDTBHHKN-UHFFFAOYSA-N
Formula: C10H5F14NO3
SMILES: O=C(NCCOC(=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]: 453.13
CAS: 70473-77-7

Physical Properties

Property code	Value	Unit	Source
gf	-2950.43	kJ/mol	Joback Method
hf	-3351.68	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	40.98	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.312		Crippen Method
mcvol	195.530	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
tb	578.93	K	Joback Method
tc	723.00	K	Joback Method
tf	399.99	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.54	J/mol×K	578.93	Joback Method
cpg	585.77	J/mol×K	602.94	Joback Method
cpg	595.22	J/mol×K	626.95	Joback Method
cpg	603.94	J/mol×K	650.97	Joback Method
cpg	611.97	J/mol×K	674.98	Joback Method
cpg	619.35	J/mol×K	698.99	Joback Method
cpg	626.14	J/mol×K	723.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70473777&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