N-Bis(trifluoroacetyl)-2-ethylbutan-1-amine

Other names: 1-[N-bis(trifluoroacetyl)]amino-2-ethylbutane
Inchi: InChI=1S/C10H13F6NO2/c1-3-6(4-2)5-17(7(18)9(11,12)13)8(19)10(14,15)16/h6H,3-5H2
InchiKey: KOBMYYWEACBTAI-UHFFFAOYSA-N
Formula: C10H13F6NO2
SMILES: CCC(CC)CN(C(=O)C(F)(F)F)C(=O)C(F)(F)F
Mol. weight [g/mol]: 293.21

Physical Properties

Property code	Value	Unit	Source
gf	-1279.36	kJ/mol	Joback Method
hf	-1606.80	kJ/mol	Joback Method
hfus	28.00	kJ/mol	Joback Method
hvap	45.51	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.902		Crippen Method
mcvol	175.500	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook
tb	537.10	K	Joback Method
tc	694.45	K	Joback Method
tf	328.17	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.77	J/mol×K	537.10	Joback Method
cpg	468.38	J/mol×K	563.33	Joback Method
cpg	480.28	J/mol×K	589.55	Joback Method
cpg	491.48	J/mol×K	615.78	Joback Method
cpg	502.02	J/mol×K	642.00	Joback Method
cpg	511.93	J/mol×K	668.23	Joback Method
cpg	521.26	J/mol×K	694.45	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=U373412&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