2,2,2-Trifluoro-N-heptyl-N-(trifluoroacetyl)acetami

Other names: 1-Bis(trifluoroacetyl)aminoheptane
Inchi: InChI=1S/C11H15F6NO2/c1-2-3-4-5-6-7-18(8(19)10(12,13)14)9(20)11(15,16)17/h2-7H2,
InchiKey: HNXMDOMUGYLAQY-UHFFFAOYSA-N
Formula: C11H15F6NO2
SMILES: CCCCCCCN(C(=O)C(F)(F)F)C(=O)C(F)(F)F
Mol. weight [g/mol]: 307.23

Physical Properties

Property code	Value	Unit	Source
gf	-1268.50	kJ/mol	Joback Method
hf	-1622.16	kJ/mol	Joback Method
hfus	34.12	kJ/mol	Joback Method
hvap	48.12	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.437		Crippen Method
mcvol	189.590	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	560.42	K	Joback Method
tc	715.14	K	Joback Method
tf	354.44	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.82	J/mol×K	560.42	Joback Method
cpg	516.69	J/mol×K	586.21	Joback Method
cpg	528.86	J/mol×K	611.99	Joback Method
cpg	540.34	J/mol×K	637.78	Joback Method
cpg	551.18	J/mol×K	663.57	Joback Method
cpg	561.40	J/mol×K	689.36	Joback Method
cpg	571.04	J/mol×K	715.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373368&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