tert-butyl-n-heptyl-amine

Inchi: InChI=1S/C11H25N/c1-5-6-7-8-9-10-12-11(2,3)4/h12H,5-10H2,1-4H3
InchiKey: YSZRBYDNFZRYSJ-UHFFFAOYSA-N
Formula: C11H25N
SMILES: CCCCCCCNC(C)(C)C
Mol. weight [g/mol]: 171.32
CAS: 78579-52-9

Physical Properties

Property code	Value	Unit	Source
gf	133.97	kJ/mol	Joback Method
hf	-225.65	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	45.22	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.345		Crippen Method
mcvol	175.830	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
tb	498.02	K	Joback Method
tc	672.68	K	Joback Method
tf	268.81	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.95	J/mol×K	498.02	Joback Method
cpg	435.28	J/mol×K	527.13	Joback Method
cpg	451.80	J/mol×K	556.24	Joback Method
cpg	467.55	J/mol×K	585.35	Joback Method
cpg	482.55	J/mol×K	614.46	Joback Method
cpg	496.83	J/mol×K	643.57	Joback Method
cpg	510.43	J/mol×K	672.68	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=C78579529&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