sec-butyl-n-octyl-amine

Inchi: InChI=1S/C11H25N/c1-4-6-7-8-9-10-12-11(3)5-2/h11-12H,4-10H2,1-3H3
InchiKey: VQCCDSKKXUNOAT-UHFFFAOYSA-N
Formula: C11H25N
SMILES: CCCCCCCNC(C)CC
Mol. weight [g/mol]: 171.32
CAS: 78579-54-1

Physical Properties

Property code	Value	Unit	Source
gf	128.69	kJ/mol	Joback Method
hf	-222.18	kJ/mol	Joback Method
hfus	25.82	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.345		Crippen Method
mcvol	175.830	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1288.00		NIST Webbook
tb	500.81	K	Joback Method
tc	669.39	K	Joback Method
tf	251.39	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.58	J/mol×K	500.81	Joback Method
cpg	432.13	J/mol×K	528.91	Joback Method
cpg	448.02	J/mol×K	557.00	Joback Method
cpg	463.26	J/mol×K	585.10	Joback Method
cpg	477.87	J/mol×K	613.19	Joback Method
cpg	491.87	J/mol×K	641.29	Joback Method
cpg	505.27	J/mol×K	669.39	Joback Method

Sources

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=C78579541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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