isopropyl-n-hexyl-amine

Inchi: InChI=1S/C9H21N/c1-4-5-6-7-8-10-9(2)3/h9-10H,4-8H2,1-3H3
InchiKey: LMJDMESPXVAQQY-UHFFFAOYSA-N
Formula: C9H21N
SMILES: CCCCCCNC(C)C
Mol. weight [g/mol]: 143.27
CAS: 78579-57-4

Physical Properties

Property code	Value	Unit	Source
gf	111.85	kJ/mol	Joback Method
hf	-180.90	kJ/mol	Joback Method
hfus	20.64	kJ/mol	Joback Method
hvap	41.68	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.565		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	991.00		NIST Webbook
tb	455.05	K	Joback Method
tc	625.99	K	Joback Method
tf	228.85	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.80	J/mol×K	455.05	Joback Method
cpg	337.76	J/mol×K	483.54	Joback Method
cpg	352.13	J/mol×K	512.03	Joback Method
cpg	365.92	J/mol×K	540.52	Joback Method
cpg	379.16	J/mol×K	569.01	Joback Method
cpg	391.84	J/mol×K	597.50	Joback Method
cpg	404.00	J/mol×K	625.99	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=C78579574&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