N,N-Diethylbenzylamine

Other names:	N-Benzyldiethylamine Benzenemethanamine, N,N-diethyl- Benzylamine, N,N-diethyl- Benzyldiethylamine Diethylbenzylamine
Inchi:	InChI=1S/C11H17N/c1-3-12(4-2)10-11-8-6-5-7-9-11/h5-9H,3-4,10H2,1-2H3
InchiKey:	ZWRDBWDXRLPESY-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CCN(CC)Cc1ccccc1
Mol. weight [g/mol]:	163.26
CAS:	772-54-3

Physical Properties

Property code	Value	Unit	Source
gf	264.93	kJ/mol	Joback Method
hf	33.69	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.528		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
rinpol	1182.30		NIST Webbook
rinpol	1173.00		NIST Webbook
tb	484.50 ± 0.50	K	NIST Webbook
tc	689.53	K	Joback Method
tf	272.62	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.37	J/mol×K	490.20	Joback Method
cpg	350.20	J/mol×K	523.42	Joback Method

cpg	366.07	J/mol×K	556.64	Joback Method
cpg	381.03	J/mol×K	589.86	Joback Method
cpg	395.11	J/mol×K	623.09	Joback Method
cpg	408.37	J/mol×K	656.31	Joback Method
cpg	420.83	J/mol×K	689.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.00	K	2.00	NIST Webbook

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=C772543&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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