

DIMETHYLHEPTYLAMINE

Other names:	Dimethyl(n-heptyl)amine N,N-dimethylheptylamine
Inchi:	InChI=1S/C9H21N/c1-4-5-6-7-8-9-10(2)3/h4-9H2,1-3H3
InchiKey:	LSICDRUYCNGRIF-UHFFFAOYSA-N
Formula:	C9H21N
SMILES:	CCCCCCC(C)N
Mol. weight [g/mol]:	143.27
CAS:	5277-11-2

Physical Properties

Property code	Value	Unit	Source
af	0.4688		Cheméo Relay (1.0)
gf	135.68	kJ/mol	Joback Method
hf	-157.77	kJ/mol	Cheméo Relay (1.0)
hfus	22.09	kJ/mol	Joback Method
hvap	46.99	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-2.44		Cheméo Relay (1.0)
logp	2.518		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
tb	443.15 ± 3.00	K	NIST Webbook
tb	445.15 ± 3.00	K	NIST Webbook
tc	604.35	K	Cheméo Relay (1.0)
tf	205.56	K	Cheméo Relay (1.0)
vc	0.581	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.35	J/mol×K	417.76	Joback Method
cpg	318.41	J/mol×K	444.73	Joback Method

cpg	332.88	J/mol×K	471.71	Joback Method
cpg	346.79	J/mol×K	498.68	Joback Method
cpg	360.15	J/mol×K	525.66	Joback Method
cpg	372.97	J/mol×K	552.63	Joback Method
cpg	385.27	J/mol×K	579.60	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58840e+01
Coeff. B	-4.26123e+03
Coeff. C	-6.49020e+01
Temperature range (K), min.	338.12
Temperature range (K), max.	467.95

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5277112&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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