DIDECYLAMINE

Other names: 1-Decanamine, N-decyl-
Armeen 2-10
Radiamine 6310
Inchi: InChI=1S/C20H43N/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h21H,3-20
InchiKey: GMTCPFCMAHMEMT-UHFFFAOYSA-N
Formula: C20H43N
SMILES: CCCCCCCCCCNCCCCCCCCCC
Mol. weight [g/mol]: 297.57
CAS: 1120-49-6

Physical Properties

Property code	Value	Unit	Source
af	0.9188		Cheméo Relay (1.0)
gf	206.91	kJ/mol	Joback Method
hf	-421.07	kJ/mol	Cheméo Relay (1.0)
hfus	52.65	kJ/mol	Joback Method
hvap	98.85	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-6.96		Cheméo Relay (1.0)
logp	6.857		Crippen Method
mcvol	302.640	ml/mol	McGowan Method
pc	1024.00	kPa	Joback Method
rinpol	2142.00		NIST Webbook
tb	637.15 ± 3.00	K	NIST Webbook
tc	763.12	K	Cheméo Relay (1.0)
tf	314.65 ± 1.00	K	NIST Webbook
tf	305.75 ± 1.00	K	NIST Webbook
tf	319.65 ± 3.00	K	NIST Webbook
tf	305.75 ± 0.50	K	NIST Webbook
tf	315.40 ± 2.00	K	NIST Webbook
tf	320.65 ± 5.00	K	NIST Webbook
tf	321.15 ± 5.00	K	NIST Webbook
vc	1.200	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.14	J/mol×K	707.17	Joback Method
cpg	931.80	J/mol×K	734.88	Joback Method
cpg	951.55	J/mol×K	762.59	Joback Method
cpg	970.43	J/mol×K	790.30	Joback Method
cpg	988.46	J/mol×K	818.01	Joback Method
cpg	1005.68	J/mol×K	845.72	Joback Method
cpg	1022.11	J/mol×K	873.43	Joback Method
hvapt	70.90	kJ/mol	605.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	452.70	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53657e+01
Coeff. B	-5.59144e+03
Coeff. C	-1.16888e+02
Temperature range (K), min.	487.72
Temperature range (K), max.	673.02

Sources

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):

Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120496&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume