TRIS(2-METHYLALLYL)AMINE

Other names: (CH2=C(CH3)CH2)3N
2-Propen-1-amine, 2-methyl-N,N-bis(2-methyl-2-propenyl)-
Inchi: InChI=1S/C12H21N/c1-10(2)7-13(8-11(3)4)9-12(5)6/h1,3,5,7-9H2,2,4,6H3
InchiKey: FXBJYRVIFGLPBC-UHFFFAOYSA-N
Formula: C12H21N
SMILES: C=C(C)CN(CC(=C)C)CC(=C)C
Mol. weight [g/mol]: 179.31

Physical Properties

Property code	Value	Unit	Source
affp	980.20	kJ/mol	NIST Webbook
basg	949.40	kJ/mol	NIST Webbook
hf	35.78	kJ/mol	Cheméo Relay (1.0)
hfus	22.09	kJ/mol	Joback Method
hvap	55.66	kJ/mol	Cheméo Relay (1.0)
ie	7.80	eV	NIST Webbook
log10ws	-2.96		Cheméo Relay (1.0)
logp	3.017		Crippen Method
mcvol	177.020	ml/mol	McGowan Method
tb	473.48	K	Cheméo Relay (1.0)
tc	635.10	K	Cheméo Relay (1.0)
tf	245.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.32	J/mol×K	476.08	Joback Method
cpg	404.17	J/mol×K	505.69	Joback Method
cpg	420.19	J/mol×K	535.30	Joback Method
cpg	435.41	J/mol×K	564.91	Joback Method
cpg	449.88	J/mol×K	594.52	Joback Method
cpg	463.62	J/mol×K	624.13	Joback Method
cpg	476.67	J/mol×K	653.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	2.00	NIST Webbook

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6321400&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point