propylamyl-amine

Inchi: InChI=1S/C8H19N/c1-3-5-6-8-9-7-4-2/h9H,3-8H2,1-2H3
InchiKey: GFAQQAUTKWCQHA-UHFFFAOYSA-N
Formula: C8H19N
SMILES: CCCCCNCCC
Mol. weight [g/mol]: 129.24
CAS: 20193-22-0

Physical Properties

Property code	Value	Unit	Source
af	0.4893		Cheméo Relay (1.0)
gf	105.87	kJ/mol	Joback Method
hf	-161.02	kJ/mol	Cheméo Relay (1.0)
hfus	21.57	kJ/mol	Joback Method
hvap	48.17	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-1.59		Cheméo Relay (1.0)
logp	2.176		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
tb	430.18	K	Cheméo Relay (1.0)
tc	597.26	K	Cheméo Relay (1.0)
tf	221.02	K	Cheméo Relay (1.0)
vc	0.518	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-5.59400e+00
Coeff. B	8.40040e-01

Coeff. C	-4.60000e-04
Coeff. D	9.45000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20193220&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
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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