2-methylphenethylamine

Inchi: InChI=1S/C9H13N/c1-8-4-2-3-5-9(8)6-7-10/h2-5H,6-7,10H2,1H3
InchiKey: OWOUKRYOZIZVFK-UHFFFAOYSA-N
Formula: C9H13N
SMILES: Cc1ccccc1CCN
Mol. weight [g/mol]: 135.21
CAS: 55755-16-3

Physical Properties

Property code	Value	Unit	Source
af	0.4751		Cheméo Relay (1.0)
gf	194.13	kJ/mol	Joback Method
hf	26.73	kJ/mol	Cheméo Relay (1.0)
hfus	17.92	kJ/mol	Joback Method
hvap	60.44	kJ/mol	Cheméo Relay (1.0)
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-1.57		Cheméo Relay (1.0)
logp	1.496		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	495.52	K	Cheméo Relay (1.0)
tc	714.10	K	Cheméo Relay (1.0)
tf	296.89	K	Cheméo Relay (1.0)
vc	0.431	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.53	J/mol×K	509.51	Joback Method
cpg	285.22	J/mol×K	546.28	Joback Method
cpg	298.11	J/mol×K	583.04	Joback Method
cpg	310.23	J/mol×K	619.81	Joback Method
cpg	321.61	J/mol×K	656.58	Joback Method
cpg	332.28	J/mol×K	693.35	Joback Method
cpg	342.28	J/mol×K	730.11	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43892e+01
Coeff. B	-3.98170e+03
Coeff. C	-7.45730e+01
Temperature range (K), min.	356.93
Temperature range (K), max.	513.20

Sources

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

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume