Ethan-d5-amine

Inchi: InChI=1S/C2H7N/c1-2-3/h2-3H2,1H3/i1D3,2D2
InchiKey: QUSNBJAOOMFDIB-ZBJDZAJPSA-N
Formula: C2H2D5N
SMILES: CCN
Mol. weight [g/mol]: 50.11
CAS: 17616-24-9

Physical Properties

Property code	Value	Unit	Source
gf	32.41	kJ/mol	Joback Method
hf	-50.82	kJ/mol	Joback Method
hfus	6.13	kJ/mol	Joback Method
hvap	30.69	kJ/mol	Joback Method
ie	9.37	eV	NIST Webbook
log10ws	-0.09		Crippen Method
logp	-0.035		Crippen Method
mcvol	49.020	ml/mol	McGowan Method
pc	5462.66	kPa	Joback Method
tb	317.69	K	Joback Method
tc	499.50	K	Joback Method
tf	195.56	K	Joback Method
vc	0.176	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	76.60	J/mol×K	317.69	Joback Method
cpg	82.00	J/mol×K	347.99	Joback Method
cpg	87.20	J/mol×K	378.29	Joback Method
cpg	92.22	J/mol×K	408.60	Joback Method
cpg	97.06	J/mol×K	438.90	Joback Method
cpg	101.72	J/mol×K	469.20	Joback Method
cpg	106.20	J/mol×K	499.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17616249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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