pentadeuteroethane

Inchi: InChI=1S/C2H6/c1-2/h1-2H3/i1D2,2D3
InchiKey: OTMSDBZUPAUEDD-KPAILUHGSA-N
Formula: C2HD5
SMILES: CC
Mol. weight [g/mol]: 35.10
CAS: 3681-30-9

Physical Properties

Property code	Value	Unit	Source
gf	-34.04	kJ/mol	Joback Method
hf	-84.61	kJ/mol	Joback Method
hfus	0.94	kJ/mol	Joback Method
hvap	20.05	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	1.026		Crippen Method
mcvol	39.040	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
tb	245.16	K	Joback Method
tc	401.63	K	Joback Method
tf	112.30	K	Joback Method
vc	0.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	43.67	J/mol×K	245.16	Joback Method
cpg	62.55	J/mol×K	375.55	Joback Method
cpg	58.97	J/mol×K	349.47	Joback Method
cpg	55.29	J/mol×K	323.39	Joback Method
cpg	51.52	J/mol×K	297.32	Joback Method
cpg	47.64	J/mol×K	271.24	Joback Method
cpg	66.03	J/mol×K	401.63	Joback Method
dvisc	0.0001008	Pa×s	245.16	Joback Method
dvisc	0.0001234	Pa×s	223.02	Joback Method

dvisc	0.0001579	Pa×s	200.87	Joback Method
dvisc	0.0002148	Pa×s	178.73	Joback Method
dvisc	0.0003187	Pa×s	156.59	Joback Method
dvisc	0.0005385	Pa×s	134.44	Joback Method
dvisc	0.0011192	Pa×s	112.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3681309&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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