

Ethyl radical-1,1-d2

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C2H5/c1-2/h1H2,2H3/i1D2

QUPDWYMUPZLYJZ-DICFDUPASA-N

C2H3D2

[CH2]C

31.07

28882-22-6

Physical Properties

Property code	Value	Unit	Source
gf	18.34	kJ/mol	Joback Method
hf	-28.80	kJ/mol	Joback Method
hfus	2.62	kJ/mol	Joback Method
hvap	19.90	kJ/mol	Joback Method
ie	8.38 ± 0.02	eV	NIST Webbook
log10ws	-0.27		Crippen Method
logp	0.840		Crippen Method
mcvol	36.890	ml/mol	McGowan Method
pc	5359.18	kPa	Joback Method
tb	244.46	K	Joback Method
tc	397.65	K	Joback Method
tf	128.67	K	Joback Method
vc	0.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	37.54	J/mol×K	244.46	Joback Method
cpg	41.90	J/mol×K	269.99	Joback Method
cpg	46.00	J/mol×K	295.52	Joback Method
cpg	49.86	J/mol×K	321.06	Joback Method
cpg	53.49	J/mol×K	346.59	Joback Method
cpg	56.91	J/mol×K	372.12	Joback Method
cpg	60.12	J/mol×K	397.65	Joback Method
dvisc	0.0000824	Pa×s	128.67	Joback Method

dvisc	0.0000788	Pa×s	147.97	Joback Method
dvisc	0.0000761	Pa×s	167.27	Joback Method
dvisc	0.0000740	Pa×s	186.56	Joback Method
dvisc	0.0000724	Pa×s	205.86	Joback Method
dvisc	0.0000710	Pa×s	225.16	Joback Method
dvisc	0.0000699	Pa×s	244.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28882226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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

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