2-C2H5-Hexane-d13

Inchi: InChI=1S/C8H18/c1-4-6-7-8(3)5-2/h8H,4-7H2,1-3H3/i1D3,3D3,4D2,6D2,7D2,8D
InchiKey: LAIUFBWHERIJIH-IVPOXXCHSA-N
Formula: C8H5D13
SMILES: CCCCC(C)CC
Mol. weight [g/mol]: 127.31

Physical Properties

Property code	Value	Unit	Source
gf	14.04	kJ/mol	Joback Method
hf	-213.73	kJ/mol	Joback Method
hfus	12.95	kJ/mol	Joback Method
hvap	33.01	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	3.223		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	763.71		NIST Webbook
rinpol	763.71		NIST Webbook
tb	382.00	K	Joback Method
tc	549.20	K	Joback Method
tf	164.92	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.14	J/mol×K	382.00	Joback Method
cpg	245.53	J/mol×K	409.87	Joback Method
cpg	258.44	J/mol×K	437.73	Joback Method
cpg	270.88	J/mol×K	465.60	Joback Method
cpg	282.86	J/mol×K	493.46	Joback Method
cpg	294.38	J/mol×K	521.33	Joback Method
cpg	305.46	J/mol×K	549.20	Joback Method
dvisc	0.0105616	Pa×s	164.92	Joback Method

dvisc	0.0031758	Pa×s	201.10	Joback Method
dvisc	0.0013776	Pa×s	237.28	Joback Method
dvisc	0.0007454	Pa×s	273.46	Joback Method
dvisc	0.0004656	Pa×s	309.64	Joback Method
dvisc	0.0003209	Pa×s	345.82	Joback Method
dvisc	0.0002373	Pa×s	382.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136526&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume