Propane-d8

Inchi: InChI=1S/C3H8/c1-3-2/h3H2,1-2H3/i1D3,2D3,3D2
InchiKey: ATUOYWHBWRKTHZ-AUOAYUKBSA-N
Formula: C3D8
SMILES: CCC
Mol. weight [g/mol]: 52.14
CAS: 2875-94-7

Physical Properties

Property code	Value	Unit	Source
gf	-25.62	kJ/mol	Joback Method
hf	-105.25	kJ/mol	Joback Method
hfus	3.53	kJ/mol	Joback Method
hvap	22.27	kJ/mol	Joback Method
ie	11.40	eV	NIST Webbook
log10ws	-1.08		Crippen Method
logp	1.416		Crippen Method
mcvol	53.130	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	268.04	K	Joback Method
tc	427.34	K	Joback Method
tf	123.57	K	Joback Method
vc	0.203	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	68.04	J/mol×K	268.04	Joback Method
cpg	95.11	J/mol×K	400.79	Joback Method
cpg	90.02	J/mol×K	374.24	Joback Method
cpg	84.77	J/mol×K	347.69	Joback Method
cpg	79.35	J/mol×K	321.14	Joback Method
cpg	73.78	J/mol×K	294.59	Joback Method
cpg	100.05	J/mol×K	427.34	Joback Method
dvisc	0.0001447	Pa×s	268.04	Joback Method

dvisc	0.0001801	Pa×s	243.96	Joback Method
dvisc	0.0002350	Pa×s	219.88	Joback Method
dvisc	0.0003273	Pa×s	195.80	Joback Method
dvisc	0.0005005	Pa×s	171.73	Joback Method
dvisc	0.0008789	Pa×s	147.65	Joback Method
dvisc	0.0019221	Pa×s	123.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2875947&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
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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