Propyne-d4

Inchi: InChI=1S/C3H4/c1-3-2/h1H,2H3/i1D,2D3
InchiKey: MWWATHDPGQKSAR-BMQYTIHCSA-N
Formula: C3D4
SMILES: C#CC
Mol. weight [g/mol]: 44.09
CAS: 6111-63-3

Physical Properties

Property code	Value	Unit	Source
gf	197.45	kJ/mol	Joback Method
hf	186.65	kJ/mol	Joback Method
hfus	6.50	kJ/mol	Joback Method
hvap	22.13	kJ/mol	Joback Method
ie	10.38	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	0.639		Crippen Method
mcvol	44.530	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	258.16	K	Joback Method
tc	428.99	K	Joback Method
tf	170.54	K	Joback Method
vc	0.166	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	55.98	J/mol×K	258.16	Joback Method
cpg	59.70	J/mol×K	286.63	Joback Method
cpg	63.26	J/mol×K	315.10	Joback Method
cpg	66.67	J/mol×K	343.57	Joback Method
cpg	69.94	J/mol×K	372.05	Joback Method
cpg	73.06	J/mol×K	400.52	Joback Method
cpg	76.04	J/mol×K	428.99	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=C6111633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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