Butadiyne-d2

Inchi: InChI=1S/C4H2/c1-3-4-2/h1-2H/i1D,2D
InchiKey: LLCSWKVOHICRDD-QDNHWIQGSA-N
Formula: C4D2
SMILES: C#CC#C
Mol. weight [g/mol]: 52.07
CAS: 16954-96-4

Physical Properties

Property code	Value	Unit	Source
gf	428.94	kJ/mol	Joback Method
hf	457.91	kJ/mol	Joback Method
hfus	12.07	kJ/mol	Joback Method
hvap	24.21	kJ/mol	Joback Method
ie	10.18 ± 0.00	eV	NIST Webbook
ie	10.18 ± 0.01	eV	NIST Webbook
log10ws	-1.09		Crippen Method
logp	0.253		Crippen Method
mcvol	50.020	ml/mol	McGowan Method
pc	5862.92	kPa	Joback Method
tb	271.16	K	Joback Method
tc	457.28	K	Joback Method
tf	228.78	K	Joback Method
vc	0.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	67.77	J/mol×K	271.16	Joback Method
cpg	71.10	J/mol×K	302.18	Joback Method
cpg	74.21	J/mol×K	333.20	Joback Method
cpg	77.10	J/mol×K	364.22	Joback Method
cpg	79.79	J/mol×K	395.24	Joback Method
cpg	82.29	J/mol×K	426.26	Joback Method
cpg	84.61	J/mol×K	457.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16954964&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
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