

(E)-2-Butene-d8

Inchi:	InChI=1S/C4H8/c1-3-4-2/h3-4H,1-2H3/b4-3+/i1D3,2D3,3D,4D
InchiKey:	IAQRGUVFOMOMEM-BDYLZKADSA-N
Formula:	C4D8
SMILES:	CC=CC
Mol. weight [g/mol]:	64.16
CAS:	1517-55-1

Physical Properties

Property code	Value	Unit	Source
gf	63.02	kJ/mol	Joback Method
hf	-8.67	kJ/mol	Joback Method
hfus	6.32	kJ/mol	Joback Method
hvap	24.46	kJ/mol	Joback Method
ie	9.17	eV	NIST Webbook
log10ws	-1.35		Crippen Method
logp	1.582		Crippen Method
mcvol	62.920	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	295.08	K	Joback Method
tc	466.02	K	Joback Method
tf	129.76	K	Joback Method
vc	0.239	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	82.22	J/mol×K	295.08	Joback Method
cpg	115.64	J/mol×K	437.53	Joback Method
cpg	109.55	J/mol×K	409.04	Joback Method
cpg	103.17	J/mol×K	380.55	Joback Method
cpg	96.50	J/mol×K	352.06	Joback Method
cpg	89.52	J/mol×K	323.57	Joback Method
cpg	121.46	J/mol×K	466.02	Joback Method
dvisc	0.0001436	Pa×s	295.08	Joback Method

dvisc	0.0001810	Pa×s	267.53	Joback Method
dvisc	0.0002406	Pa×s	239.97	Joback Method
dvisc	0.0003443	Pa×s	212.42	Joback Method
dvisc	0.0005483	Pa×s	184.87	Joback Method
dvisc	0.0010280	Pa×s	157.31	Joback Method
dvisc	0.0025167	Pa×s	129.76	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=C1517551&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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