1,2,3-Butatriene, 1-ethoxy

Inchi: InChI=1S/C6H8O/c1-3-5-6-7-4-2/h6H,1,4H2,2H3
InchiKey: DGJJASURVQPVJG-UHFFFAOYSA-N
Formula: C6H8O
SMILES: C=C=C=COCC
Mol. weight [g/mol]: 96.13
CAS: 26842-75-1

Physical Properties

Property code	Value	Unit	Source
gf	239.04	kJ/mol	Joback Method
hf	151.60	kJ/mol	Joback Method
hfus	15.46	kJ/mol	Joback Method
hvap	31.56	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.477		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
tb	362.32	K	Joback Method
tc	553.87	K	Joback Method
tf	190.87	K	Joback Method
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.94	J/mol×K	362.32	Joback Method
cpg	159.91	J/mol×K	394.25	Joback Method
cpg	166.84	J/mol×K	426.17	Joback Method
cpg	173.70	J/mol×K	458.10	Joback Method
cpg	180.48	J/mol×K	490.02	Joback Method
cpg	187.14	J/mol×K	521.95	Joback Method
cpg	193.68	J/mol×K	553.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26842751&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume