trans-3-Methoxy-2-pentene

Inchi: InChI=1S/C6H12O/c1-4-6(5-2)7-3/h4H,5H2,1-3H3/b6-4+
InchiKey: SDCXDHFQQVVBEN-GQCTYLIASA-N
Formula: C6H12O
SMILES: CC=C(CC)OC
Mol. weight [g/mol]: 100.16
CAS: 53260-03-0

Physical Properties

Property code	Value	Unit	Source
gf	-33.69	kJ/mol	Joback Method
hf	-191.96	kJ/mol	Joback Method
hfus	11.38	kJ/mol	Joback Method
hvap	31.40	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.947		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
tb	363.14	K	Joback Method
tc	540.00	K	Joback Method
tf	160.57	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.72	J/mol×K	363.14	Joback Method
cpg	177.87	J/mol×K	392.62	Joback Method
cpg	187.64	J/mol×K	422.09	Joback Method
cpg	197.05	J/mol×K	451.57	Joback Method
cpg	206.10	J/mol×K	481.05	Joback Method
cpg	214.81	J/mol×K	510.52	Joback Method
cpg	223.18	J/mol×K	540.00	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=C53260030&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
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