C11H20O2

Inchi: InChI=1S/C11H20O2/c1-4-7-8-9-10-11(12-5-2)13-6-3/h11H,4-8H2,1-3H3
InchiKey: NKXTVBJJMIROGV-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: CCCCC#CC(OCC)OCC
Mol. weight [g/mol]: 184.28
CAS: 18232-30-9

Physical Properties

Property code	Value	Unit	Source
gf	32.10	kJ/mol	Joback Method
hf	-267.79	kJ/mol	Joback Method
hfus	26.22	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.579		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
tb	504.48	K	Joback Method
tc	689.45	K	Joback Method
tf	349.29	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.97	J/mol×K	504.48	Joback Method
cpg	399.23	J/mol×K	535.31	Joback Method
cpg	413.96	J/mol×K	566.14	Joback Method
cpg	428.15	J/mol×K	596.96	Joback Method
cpg	441.80	J/mol×K	627.79	Joback Method
cpg	454.91	J/mol×K	658.62	Joback Method
cpg	467.47	J/mol×K	689.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18232309&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
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