trans-Shisool

Inchi: InChI=1S/C10H18O/c1-8(2)10-5-3-9(7-11)4-6-10/h9-11H,1,3-7H2,2H3/t9-,10-
InchiKey: GMYHXOPIKMGWOM-MGCOHNPYSA-N
Formula: C10H18O
SMILES: C=C(C)C1CCC(CO)CC1
Mol. weight [g/mol]: 154.25
CAS: 22451-48-5

Physical Properties

Property code	Value	Unit	Source
gf	-7.47	kJ/mol	Joback Method
hf	-252.34	kJ/mol	Joback Method
hfus	16.06	kJ/mol	Joback Method
hvap	54.06	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.361		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1248.00		NIST Webbook
rinpol	1248.00		NIST Webbook
tb	531.82	K	Joback Method
tc	724.69	K	Joback Method
tf	250.70	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.92	J/mol×K	531.82	Joback Method
cpg	366.34	J/mol×K	563.96	Joback Method
cpg	381.93	J/mol×K	596.11	Joback Method
cpg	396.71	J/mol×K	628.25	Joback Method
cpg	410.71	J/mol×K	660.40	Joback Method
cpg	423.96	J/mol×K	692.54	Joback Method
cpg	436.46	J/mol×K	724.69	Joback Method

Sources

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=C22451485&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume