trans-p-Mentha-8-methylthio-3-one

Inchi: InChI=1S/C11H20OS/c1-8-5-6-9(10(12)7-8)11(2,3)13-4/h8-9H,5-7H2,1-4H3/t8-,9-/m0/s1
InchiKey: HJFSNLWDUINFTB-IUCAKERBSA-N
Formula: C11H20OS
SMILES: CSC(C)(C)C1CCC(C)CC1=O
Mol. weight [g/mol]: 200.34

Physical Properties

Property code	Value	Unit	Source
gf	-28.15	kJ/mol	Joback Method
hf	-340.97	kJ/mol	Joback Method
hfus	13.38	kJ/mol	Joback Method
hvap	49.97	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.133		Crippen Method
mcvol	172.910	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
ripol	1916.00		NIST Webbook
ripol	1916.00		NIST Webbook
tb	599.33	K	Joback Method
tc	842.49	K	Joback Method
tf	321.91	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.63	J/mol×K	599.33	Joback Method
cpg	475.07	J/mol×K	639.86	Joback Method
cpg	495.12	J/mol×K	680.38	Joback Method
cpg	513.79	J/mol×K	720.91	Joback Method
cpg	531.08	J/mol×K	761.44	Joback Method
cpg	547.01	J/mol×K	801.97	Joback Method
cpg	561.60	J/mol×K	842.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R620967&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume