(1S,3aR,4R,8R,8aS)-1-Isopropyl-3a-methyl-7-meth

Inchi: InChI=1S/C15H24S/c1-9(2)11-7-8-15(4)12-6-5-10(3)14(16-12)13(11)15/h9,11-14H,3,5-8
InchiKey: HVLGGQYBXOJMLO-UHFFFAOYSA-N
Formula: C15H24S
SMILES: C=C1CCC2SC1C1C(C(C)C)CCC21C
Mol. weight [g/mol]: 236.42
CAS: 72445-42-2

Physical Properties

Property code	Value	Unit	Source
gf	303.06	kJ/mol	Joback Method
hf	-48.07	kJ/mol	Joback Method
hfus	19.63	kJ/mol	Joback Method
hvap	52.88	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.509		Crippen Method
mcvol	201.680	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1743.50		NIST Webbook
tb	608.81	K	Joback Method
tc	839.95	K	Joback Method
tf	403.14	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.71	J/mol×K	608.81	Joback Method
cpg	582.66	J/mol×K	647.33	Joback Method
cpg	604.14	J/mol×K	685.86	Joback Method
cpg	624.36	J/mol×K	724.38	Joback Method
cpg	643.55	J/mol×K	762.90	Joback Method
cpg	661.91	J/mol×K	801.43	Joback Method
cpg	679.65	J/mol×K	839.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72445422&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume