(1-adamantyl)2CS

Inchi: InChI=1S/C21H30S/c22-19(20-7-13-1-14(8-20)3-15(2-13)9-20)21-10-16-4-17(11-21)6-18
InchiKey: PRGACUHWUBEYRP-UHFFFAOYSA-N
Formula: C21H30S
SMILES: S=C(C12CC3CC(CC(C3)C1)C2)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 314.53
CAS: 73509-04-3

Physical Properties

Property code	Value	Unit	Source
affp	912.10	kJ/mol	NIST Webbook
basg	882.40	kJ/mol	NIST Webbook
gf	556.90	kJ/mol	Joback Method
hf	84.01	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	65.97	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.789		Crippen Method
mcvol	253.640	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
tb	790.04	K	Joback Method
tc	1052.54	K	Joback Method
tf	500.62	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.93	J/mol×K	790.04	Joback Method
cpg	895.47	J/mol×K	833.79	Joback Method
cpg	923.16	J/mol×K	877.54	Joback Method
cpg	951.73	J/mol×K	921.29	Joback Method
cpg	981.89	J/mol×K	965.04	Joback Method
cpg	1014.34	J/mol×K	1008.79	Joback Method
cpg	1049.81	J/mol×K	1052.54	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=C73509043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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