N-heptylsulfonylpropanone

Inchi: InChI=1S/C10H20O3S/c1-3-4-5-6-7-8-14(12,13)9-10(2)11/h3-9H2,1-2H3
InchiKey: RZYNZNVSZNDITD-UHFFFAOYSA-N
Formula: C10H20O3S
SMILES: CCCCCCCS(=O)(=O)CC(C)=O
Mol. weight [g/mol]: 220.33
CAS: 94045-48-4

Physical Properties

Property code	Value	Unit	Source
gf	-564.14	kJ/mol	Joback Method
hf	-815.66	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	63.23	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.961		Crippen Method
mcvol	181.420	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	529.85	K	Joback Method
tc	699.46	K	Joback Method
tf	290.95	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.67	J/mol×K	529.85	Joback Method
cpg	440.27	J/mol×K	558.12	Joback Method
cpg	454.28	J/mol×K	586.39	Joback Method
cpg	467.69	J/mol×K	614.65	Joback Method
cpg	480.51	J/mol×K	642.92	Joback Method
cpg	492.74	J/mol×K	671.19	Joback Method
cpg	504.39	J/mol×K	699.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94045484&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