Octane, 1,1'-sulfonylbis-

Other names: dioctyl sulfone
Inchi: InChI=1S/C16H34O2S/c1-3-5-7-9-11-13-15-19(17,18)16-14-12-10-8-6-4-2/h3-16H2,1-2H
InchiKey: TZPCGEVFZZYCIY-UHFFFAOYSA-N
Formula: C16H34O2S
SMILES: CCCCCCCCS(=O)(=O)CCCCCCCC
Mol. weight [g/mol]: 290.50
CAS: 7726-20-7

Physical Properties

Property code	Value	Unit	Source
gf	-384.70	kJ/mol	Joback Method
hf	-826.92	kJ/mol	Joback Method
hfus	48.57	kJ/mol	Joback Method
hvap	69.84	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	5.122		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
tb	613.26	K	Joback Method
tc	771.84	K	Joback Method
tf	348.00 ± 3.00	K	NIST Webbook
tf	352.00 ± 4.00	K	NIST Webbook
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.72	J/mol×K	613.26	Joback Method
cpg	728.63	J/mol×K	639.69	Joback Method
cpg	746.76	J/mol×K	666.12	Joback Method
cpg	764.12	J/mol×K	692.55	Joback Method
cpg	780.73	J/mol×K	718.98	Joback Method
cpg	796.60	J/mol×K	745.41	Joback Method
cpg	811.74	J/mol×K	771.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7726207&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume