Diisobutyl sulfite

Inchi: InChI=1S/C8H18O3S/c1-7(2)5-10-12(9)11-6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey: SYKANJDVMZPZMM-UHFFFAOYSA-N
Formula: C8H18O3S
SMILES: CC(C)COS(=O)OCC(C)C
Mol. weight [g/mol]: 194.30
CAS: 18748-27-1

Physical Properties

Property code	Value	Unit	Source
hf	-651.67	kJ/mol	Cheméo Relay (1.0)
hfus	19.56	kJ/mol	Joback Method
hvap	59.72	kJ/mol	Cheméo Relay (1.0)
ie	9.79	eV	Cheméo Relay (1.0)
logp	1.910		Crippen Method
mcvol	157.540	ml/mol	McGowan Method
tb	491.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.38	J/mol×K	484.68	Joback Method
cpg	363.36	J/mol×K	514.65	Joback Method
cpg	376.89	J/mol×K	544.63	Joback Method
cpg	389.95	J/mol×K	574.60	Joback Method
cpg	402.53	J/mol×K	604.57	Joback Method
cpg	414.61	J/mol×K	634.55	Joback Method
cpg	426.20	J/mol×K	664.52	Joback Method

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.15641e+01
Coeff. B	-3.04526e+03
Coeff. C	-7.54660e+01
Temperature range (K), min.	345.52
Temperature range (K), max.	562.51

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature