Ethyl n-propyl sulphone

Inchi: InChI=1S/C5H12O2S/c1-3-5-8(6,7)4-2/h3-5H2,1-2H3
InchiKey: URDYJNJREUFXGD-UHFFFAOYSA-N
Formula: C5H12O2S
SMILES: CCCS(=O)(=O)CC
Mol. weight [g/mol]: 136.22

Physical Properties

Property code	Value	Unit	Source
hf	-442.41	kJ/mol	Cheméo Relay (1.0)
hfus	20.08	kJ/mol	Joback Method
hvap	79.46	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-0.92		Cheméo Relay (1.0)
logp	0.831		Crippen Method
mcvol	109.400	ml/mol	McGowan Method
tb	512.86	K	Cheméo Relay (1.0)
tf	296.20 ± 0.50	K	NIST Webbook
tf	266.00 ± 5.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.29	J/mol×K	361.58	Joback Method
cpg	202.32	J/mol×K	388.75	Joback Method
cpg	212.05	J/mol×K	415.91	Joback Method
cpg	221.49	J/mol×K	443.08	Joback Method
cpg	230.62	J/mol×K	470.24	Joback Method
cpg	239.46	J/mol×K	497.41	Joback Method
cpg	247.99	J/mol×K	524.57	Joback Method

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31110653&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point