Ethyl n-propyl sulfone

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]: 136.21
CAS: 31110-65-3

Physical Properties

Property code	Value	Unit	Source
gf	-477.32	kJ/mol	Joback Method
hf	-599.88	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	45.36	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.831		Crippen Method
mcvol	109.400	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
tb	361.58	K	Joback Method
tc	524.57	K	Joback Method
tf	266.00 ± 5.00	K	NIST Webbook
tf	296.20 ± 0.50	K	NIST Webbook
vc	0.442	m3/kmol	Joback Method

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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31110653&Units=SI

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