2-ethylhexyl sulfate

Inchi: InChI=1S/C8H18O4S/c1-3-5-6-8(4-2)7-12-13(9,10)11/h8H,3-7H2,1-2H3,(H,9,10,11)/p-1
InchiKey: MHGOKSLTIUHUBF-UHFFFAOYSA-M
Formula: C8H18O4S
SMILES: CCCCC(CC)COS(=O)(=O)[O-]
Mol. weight [g/mol]: 209.29
CAS: 72214-01-8

Physical Properties

Property code	Value	Unit	Source
af	0.6503		Cheméo Relay (1.0)
hf	-822.12	kJ/mol	Cheméo Relay (1.0)
hvap	71.51	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.82		Cheméo Relay (1.0)
logp	1.680		Crippen Method
mcvol	161.260	ml/mol	McGowan Method
pc	2402.36	kPa	Cheméo Relay (1.0, beta)
tb	513.07	K	Cheméo Relay (1.0)
tc	665.07	K	Cheméo Relay (1.0)
tf	212.05	K	Cheméo Relay (1.0)
vc	0.576	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.18906e+01
Coeff. B	-3.52578e+03
Coeff. C	-8.81480e+01
Temperature range (K), min.	392.02
Temperature range (K), max.	624.05

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
hf:	Enthalpy of formation 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume