Benzoic acid, p-(methylsulfonamido)-, ethyl ester

Inchi: InChI=1S/C10H13NO4S/c1-3-15-10(12)8-4-6-9(7-5-8)11-16(2,13)14/h4-7,11H,3H2,1-2H
InchiKey: AOBNSCYTCGBVQR-UHFFFAOYSA-N
Formula: C10H13NO4S
SMILES: CCOC(=O)c1ccc(NS(C)(=O)=O)cc1
Mol. weight [g/mol]: 243.28
CAS: 7151-77-1

Physical Properties

Property code	Value	Unit	Source
gf	-476.97	kJ/mol	Joback Method
hf	-669.35	kJ/mol	Joback Method
hfus	34.57	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.235		Crippen Method
mcvol	173.510	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	634.10	K	Joback Method
tc	840.20	K	Joback Method
tf	404.78	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.10	J/mol×K	634.10	Joback Method
cpg	443.28	J/mol×K	668.45	Joback Method
cpg	455.63	J/mol×K	702.80	Joback Method
cpg	467.14	J/mol×K	737.15	Joback Method
cpg	477.82	J/mol×K	771.50	Joback Method
cpg	487.65	J/mol×K	805.85	Joback Method
cpg	496.64	J/mol×K	840.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7151771&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

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