BENZENESULFONIC ACID, 4-METHYL-, 1-METHYLETHYL ESTER

Other names: isopropyl toluene-4-sulphonate
isopropyl p-toluenesulfonate
Inchi: InChI=1S/C10H14O3S/c1-8(2)13-14(11,12)10-6-4-9(3)5-7-10/h4-8H,1-3H3
InchiKey: SDQCGKJCBWXRMK-UHFFFAOYSA-N
Formula: C10H14O3S
SMILES: Cc1ccc(S(=O)(=O)OC(C)C)cc1
Mol. weight [g/mol]: 214.29

Physical Properties

Property code	Value	Unit	Source
hf	-497.47	kJ/mol	Cheméo Relay (1.0)
hfus	24.35	kJ/mol	Joback Method
hvap	79.71	kJ/mol	Cheméo Relay (1.0)
ie	8.76	eV	Cheméo Relay (1.0)
log10ws	-2.78		Cheméo Relay (1.0)
logp	2.109		Crippen Method
mcvol	161.960	ml/mol	McGowan Method
tb	552.84	K	Cheméo Relay (1.0)
tf	314.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.85	J/mol×K	529.62	Joback Method
cpg	376.78	J/mol×K	563.32	Joback Method
cpg	390.95	J/mol×K	597.01	Joback Method
cpg	404.38	J/mol×K	630.71	Joback Method
cpg	417.06	J/mol×K	664.41	Joback Method
cpg	428.99	J/mol×K	698.11	Joback Method
cpg	440.17	J/mol×K	731.80	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2307699&Units=SI
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):	

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