

Gamma-chloro-n-propyl-p-toluene sulfonate

Inchi:	InChI=1S/C10H13ClO3S/c1-9-3-5-10(6-4-9)15(12,13)14-8-2-7-11/h3-6H,2,7-8H2,1H3
InchiKey:	NQCQVNHNLNXCSPY-UHFFFAOYSA-N
Formula:	C10H13ClO3S
SMILES:	Cc1ccc(S(=O)(=O)OCCCCl)cc1
Mol. weight [g/mol]:	248.73
CAS:	632-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-449.37	kJ/mol	Joback Method
hf	-625.98	kJ/mol	Joback Method
hfus	32.07	kJ/mol	Joback Method
hvap	66.22	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.329		Crippen Method
mcvol	174.200	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	567.49	K	Joback Method
tc	770.00	K	Joback Method
tf	332.11	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.83	J/mol×K	567.49	Joback Method
cpg	403.62	J/mol×K	601.24	Joback Method
cpg	416.65	J/mol×K	634.99	Joback Method
cpg	428.94	J/mol×K	668.75	Joback Method
cpg	440.47	J/mol×K	702.50	Joback Method
cpg	451.26	J/mol×K	736.25	Joback Method
cpg	461.29	J/mol×K	770.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C632020&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

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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