4-(Methylthio)benzoic acid, 3-chlorobenzyl ester

Inchi: InChI=1S/C15H13ClO2S/c1-19-14-7-5-12(6-8-14)15(17)18-10-11-3-2-4-13(16)9-11/h2-9
InchiKey: SVXKXQHRVSGYOJ-UHFFFAOYSA-N
Formula: C15H13ClO2S
SMILES: CSc1ccc(C(=O)OCc2cccc(Cl)c2)cc1
Mol. weight [g/mol]: 292.78

Physical Properties

Property code	Value	Unit	Source
gf	68.25	kJ/mol	Joback Method
hf	-121.48	kJ/mol	Joback Method
hfus	33.02	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.419		Crippen Method
mcvol	210.720	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	788.42	K	Joback Method
tc	1044.88	K	Joback Method
tf	473.17	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.93	J/mol×K	788.42	Joback Method
cpg	553.03	J/mol×K	831.16	Joback Method
cpg	564.83	J/mol×K	873.91	Joback Method
cpg	575.37	J/mol×K	916.65	Joback Method
cpg	584.69	J/mol×K	959.39	Joback Method
cpg	592.82	J/mol×K	1002.14	Joback Method
cpg	599.81	J/mol×K	1044.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375063&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume