p-Cresyl isotiglate

Inchi: InChI=1S/C12H14O2/c1-4-10(3)12(13)14-11-7-5-9(2)6-8-11/h4-8H,1-3H3/b10-4-
InchiKey: LCQKGXUGNAWHAK-WMZJFQQLSA-N
Formula: C12H14O2
SMILES: CC=C(C)C(=O)Oc1ccc(C)cc1
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	-9.31	kJ/mol	Joback Method
hf	-203.32	kJ/mol	Joback Method
hfus	22.17	kJ/mol	Joback Method
hvap	54.44	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.867		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1482.00		NIST Webbook
ripol	2011.00		NIST Webbook
tb	585.95	K	Joback Method
tc	805.80	K	Joback Method
tf	317.06	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.70	J/mol×K	585.95	Joback Method
cpg	388.31	J/mol×K	622.59	Joback Method
cpg	402.04	J/mol×K	659.23	Joback Method
cpg	414.91	J/mol×K	695.87	Joback Method
cpg	426.97	J/mol×K	732.52	Joback Method
cpg	438.25	J/mol×K	769.16	Joback Method
cpg	448.78	J/mol×K	805.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410136&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume