(1R,4S)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl 3-chlorobenzoate

Inchi: InChI=1S/C17H21ClO2/c1-16(2)12-7-8-17(16,3)14(10-12)20-15(19)11-5-4-6-13(18)9-11/
InchiKey: FURJZQGTPYIXDV-UHFFFAOYSA-N
Formula: C17H21ClO2
SMILES: CC1(C)C2CCC1(C)C(OC(=O)c1cccc(Cl)c1)C2
Mol. weight [g/mol]: 292.80

Physical Properties

Property code	Value	Unit	Source
gf	32.19	kJ/mol	Joback Method
hf	-300.45	kJ/mol	Joback Method
hfus	24.14	kJ/mol	Joback Method
hvap	66.99	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.712		Crippen Method
mcvol	224.590	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
tb	742.63	K	Joback Method
tc	984.98	K	Joback Method
tf	494.05	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.46	J/mol×K	742.63	Joback Method
cpg	673.02	J/mol×K	783.02	Joback Method
cpg	692.20	J/mol×K	823.41	Joback Method
cpg	711.33	J/mol×K	863.80	Joback Method
cpg	730.73	J/mol×K	904.20	Joback Method
cpg	750.75	J/mol×K	944.59	Joback Method
cpg	771.72	J/mol×K	984.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373545&Units=SI

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