(6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl 3-chlorobenzoate

Inchi: InChI=1S/C17H19ClO2/c1-17(2)13-7-6-12(15(17)9-13)10-20-16(19)11-4-3-5-14(18)8-11/
InchiKey: XNSRECQDHQFWQH-UHFFFAOYSA-N
Formula: C17H19ClO2
SMILES: CC1(C)C2CC=C(COC(=O)c3cccc(Cl)c3)C1C2
Mol. weight [g/mol]: 290.79

Physical Properties

Property code	Value	Unit	Source
gf	65.72	kJ/mol	Joback Method
hf	-249.04	kJ/mol	Joback Method
hfus	30.20	kJ/mol	Joback Method
hvap	69.41	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.489		Crippen Method
mcvol	220.290	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	751.20	K	Joback Method
tc	987.96	K	Joback Method
tf	487.67	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.79	J/mol×K	751.20	Joback Method
cpg	646.22	J/mol×K	790.66	Joback Method
cpg	662.92	J/mol×K	830.12	Joback Method
cpg	679.11	J/mol×K	869.58	Joback Method
cpg	694.98	J/mol×K	909.04	Joback Method
cpg	710.75	J/mol×K	948.50	Joback Method
cpg	726.61	J/mol×K	987.96	Joback Method

Sources

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=U373577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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