(6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C17H15F5O2/c1-17(2)8-4-3-7(9(17)5-8)6-24-16(23)10-11(18)13(20)15(22)14(2
InchiKey: NVADTXGNFOKTEH-UHFFFAOYSA-N
Formula: C17H15F5O2
SMILES: CC1(C)C2CC=C(COC(=O)c3c(F)c(F)c(F)c(F)c3F)C1C2
Mol. weight [g/mol]: 346.29

Physical Properties

Property code	Value	Unit	Source
gf	-934.92	kJ/mol	Joback Method
hf	-1259.73	kJ/mol	Joback Method
hfus	39.84	kJ/mol	Joback Method
hvap	63.58	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	4.531		Crippen Method
mcvol	216.900	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
tb	730.04	K	Joback Method
tc	925.84	K	Joback Method
tf	510.78	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.92	J/mol×K	730.04	Joback Method
cpg	651.39	J/mol×K	762.67	Joback Method
cpg	665.32	J/mol×K	795.31	Joback Method
cpg	678.79	J/mol×K	827.94	Joback Method
cpg	691.92	J/mol×K	860.57	Joback Method
cpg	704.80	J/mol×K	893.21	Joback Method
cpg	717.53	J/mol×K	925.84	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=U373605&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