Perillyl benzoate

Inchi: InChI=1S/C17H20O2/c1-13(2)15-10-8-14(9-11-15)12-19-17(18)16-6-4-3-5-7-16/h3-8,15H
InchiKey: AKJMZNHWFFRVTF-UHFFFAOYSA-N
Formula: C17H20O2
SMILES: C=C(C)C1CC=C(COC(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 256.34
CAS: 73524-02-4

Physical Properties

Property code	Value	Unit	Source
gf	94.82	kJ/mol	Joback Method
hf	-186.21	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	65.66	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.146		Crippen Method
mcvol	214.610	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	2067.50		NIST Webbook
rinpol	2067.50		NIST Webbook
tb	711.58	K	Joback Method
tc	944.42	K	Joback Method
tf	384.87	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.68	J/mol×K	711.58	Joback Method
cpg	618.36	J/mol×K	750.39	Joback Method
cpg	635.63	J/mol×K	789.19	Joback Method
cpg	651.55	J/mol×K	828.00	Joback Method
cpg	666.18	J/mol×K	866.81	Joback Method
cpg	679.57	J/mol×K	905.62	Joback Method
cpg	691.78	J/mol×K	944.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73524024&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

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