3,3,5-Trimethylcyclohexyl 2-acetoxybenzoate

Other names: Benzoic acid, 2-acetyloxy-, 3,3,5-trimethylcyclohexyl ester
Heliophan acetate
Inchi: InChI=1S/C18H24O4/c1-12-9-14(11-18(3,4)10-12)22-17(20)15-7-5-6-8-16(15)21-13(2)19
InchiKey: IBNMWGITXDVFJP-UHFFFAOYSA-N
Formula: C18H24O4
SMILES: CC(=O)Oc1ccccc1C(=O)OC1CC(C)CC(C)(C)C1
Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-260.84	kJ/mol	Joback Method
hf	-650.51	kJ/mol	Joback Method
hfus	29.28	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.983		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	2047.00		NIST Webbook
tb	805.93	K	Joback Method
tc	1035.64	K	Joback Method
tf	498.68	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.45	J/mol×K	805.93	Joback Method
cpg	777.72	J/mol×K	844.22	Joback Method
cpg	796.00	J/mol×K	882.50	Joback Method
cpg	813.42	J/mol×K	920.79	Joback Method
cpg	830.07	J/mol×K	959.07	Joback Method
cpg	846.08	J/mol×K	997.36	Joback Method
cpg	861.54	J/mol×K	1035.64	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=U373292&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