4-Piperidyl benzilate

Other names: 4-Piperidyl benzylate
Inchi: InChI=1S/C19H21NO3/c21-18(23-17-11-13-20-14-12-17)19(22,15-7-3-1-4-8-15)16-9-5-2
InchiKey: CNWMSZBRGJWEKC-UHFFFAOYSA-N
Formula: C19H21NO3
SMILES: O=C(OC1CCNCC1)C(O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 311.37
CAS: 25811-48-7

Physical Properties

Property code	Value	Unit	Source
gf	78.18	kJ/mol	Joback Method
hf	-276.08	kJ/mol	Joback Method
hfus	33.93	kJ/mol	Joback Method
hvap	94.17	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.218		Crippen Method
mcvol	243.480	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	2466.00		NIST Webbook
tb	920.82	K	Joback Method
tc	1169.25	K	Joback Method
tf	604.54	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.80	J/mol×K	920.82	Joback Method
cpg	795.34	J/mol×K	962.22	Joback Method
cpg	807.47	J/mol×K	1003.63	Joback Method
cpg	818.29	J/mol×K	1045.03	Joback Method
cpg	827.92	J/mol×K	1086.44	Joback Method
cpg	836.46	J/mol×K	1127.84	Joback Method
cpg	844.03	J/mol×K	1169.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25811487&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