

Alpha-p-n-butyl-benzhydryl-acetophenone

Inchi:	InChI=1S/C25H26O/c1-2-3-10-20-15-17-22(18-16-20)24(21-11-6-4-7-12-21)19-25(26)23
InchiKey:	SPFSVEKWCKWVLI-UHFFFAOYSA-N
Formula:	C25H26O
SMILES:	CCCCc1ccc(C(CC(=O)c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]:	342.47
CAS:	116400-85-2

Physical Properties

Property code	Value	Unit	Source
gf	355.86	kJ/mol	Joback Method
hf	20.93	kJ/mol	Joback Method
hfus	40.32	kJ/mol	Joback Method
hvap	85.09	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.434		Crippen Method
mcvol	293.400	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
tb	909.85	K	Joback Method
tc	1153.00	K	Joback Method
tf	498.22	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.21	J/molxK	909.85	Joback Method
cpg	921.69	J/molxK	950.37	Joback Method
cpg	936.82	J/molxK	990.90	Joback Method
cpg	950.73	J/molxK	1031.42	Joback Method
cpg	963.55	J/molxK	1071.95	Joback Method
cpg	975.42	J/molxK	1112.47	Joback Method
cpg	986.46	J/molxK	1153.00	Joback Method
dvisc	0.0007410	Paxs	498.22	Joback Method
dvisc	0.0003578	Paxs	566.83	Joback Method

dvisc	0.0002021	Paxs	635.43	Joback Method
dvisc	0.0001276	Paxs	704.04	Joback Method
dvisc	0.0000875	Paxs	772.64	Joback Method
dvisc	0.0000637	Paxs	841.25	Joback Method
dvisc	0.0000487	Paxs	909.85	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=C116400852&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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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