

Beta-phenyl, beta-1-naphthyl p-bromopropiophenone

Inchi:	InChI=1S/C25H19BrO/c26-21-15-13-20(14-16-21)25(27)17-24(19-7-2-1-3-8-19)23-12-6-
InchiKey:	DZSMNBIDMCHTGR-UHFFFAOYSA-N
Formula:	C25H19BrO
SMILES:	O=C(CC(c1ccccc1)c1cccc2ccccc12)c1ccc(Br)cc1
Mol. weight [g/mol]:	415.32
CAS:	5472-05-9

Physical Properties

Property code	Value	Unit	Source
gf	467.20	kJ/mol	Joback Method
hf	226.86	kJ/mol	Joback Method
hfus	42.23	kJ/mol	Joback Method
hvap	93.83	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	7.007		Crippen Method
mcvol	291.440	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
tb	999.97	K	Joback Method
tc	1274.17	K	Joback Method
tf	603.24	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.28	J/molxK	999.97	Joback Method
cpg	869.22	J/molxK	1045.67	Joback Method
cpg	882.43	J/molxK	1091.37	Joback Method
cpg	895.15	J/molxK	1137.07	Joback Method
cpg	907.62	J/molxK	1182.77	Joback Method
cpg	920.08	J/molxK	1228.47	Joback Method
cpg	932.76	J/molxK	1274.17	Joback Method
dvisc	0.0005698	Paxs	603.24	Joback Method
dvisc	0.0003525	Paxs	669.36	Joback Method

dvisc	0.0002377	Paxs	735.48	Joback Method
dvisc	0.0001711	Paxs	801.61	Joback Method
dvisc	0.0001294	Paxs	867.73	Joback Method
dvisc	0.0001019	Paxs	933.85	Joback Method
dvisc	0.0000828	Paxs	999.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5472059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
mccvol:	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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