

Ketone, 2-methoxy-1-naphthyl-beta-phenylethyl

Inchi:	InChI=1S/C20H18O2/c1-22-19-14-12-16-9-5-6-10-17(16)20(19)18(21)13-11-15-7-3-2-4-8
InchiKey:	VCIIIMBEBARQCW-UHFFFAOYSA-N
Formula:	C20H18O2
SMILES:	COc1ccc2ccccc2c1C(=O)CCc1ccccc1
Mol. weight [g/mol]:	290.36

Physical Properties

Property code	Value	Unit	Source
gf	195.81	kJ/mol	Joback Method
hf	-59.74	kJ/mol	Joback Method
hfus	34.67	kJ/mol	Joback Method
hvap	76.79	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.664		Crippen Method
mcvol	233.120	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
tb	815.59	K	Joback Method
tc	1057.88	K	Joback Method
tf	497.90	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.67	J/molxK	815.59	Joback Method
cpg	679.83	J/molxK	855.97	Joback Method
cpg	693.78	J/molxK	896.35	Joback Method
cpg	706.63	J/molxK	936.73	Joback Method
cpg	718.46	J/molxK	977.12	Joback Method
cpg	729.38	J/molxK	1017.50	Joback Method
cpg	739.47	J/molxK	1057.88	Joback Method
dvisc	0.0008505	Paxs	497.90	Joback Method
dvisc	0.0005531	Paxs	550.85	Joback Method
dvisc	0.0003879	Paxs	603.80	Joback Method

dvisc	0.0002881	Paxs	656.75	Joback Method
dvisc	0.0002236	Paxs	709.69	Joback Method
dvisc	0.0001798	Paxs	762.64	Joback Method
dvisc	0.0001487	Paxs	815.59	Joback Method

Sources

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=B6002604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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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