

3-(4-Methoxyphenyl)-1-(2-naphthyl)prop-2-en-1-one

Other names:	1-(2-Naphthyl)-3-(4-methoxyphenyl) prop-2-en-1-one
Inchi:	InChI=1S/C20H16O2/c1-22-19-11-6-15(7-12-19)8-13-20(21)18-10-9-16-4-2-3-5-17(16)14
InchiKey:	VZFRSPMIFYIXSS-MDWZMJQESA-N
Formula:	C20H16O2
SMILES:	COc1ccc(C=CC(=O)c2ccc3ccccc3c2)cc1
Mol. weight [g/mol]:	288.34
CAS:	22359-67-7

Physical Properties

Property code	Value	Unit	Source
gf	276.03	kJ/mol	Joback Method
hf	57.48	kJ/mol	Joback Method
hfus	34.87	kJ/mol	Joback Method
hvap	76.74	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	4.744		Crippen Method
mcvol	228.820	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
tb	819.75	K	Joback Method
tc	1070.61	K	Joback Method
tf	492.82	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.30	J/mol×K	819.75	Joback Method
cpg	652.99	J/mol×K	861.56	Joback Method
cpg	666.53	J/mol×K	903.37	Joback Method
cpg	679.06	J/mol×K	945.18	Joback Method
cpg	690.71	J/mol×K	986.99	Joback Method
cpg	701.59	J/mol×K	1028.80	Joback Method
cpg	711.85	J/mol×K	1070.61	Joback Method
dvisc	0.0007734	Pa×s	492.82	Joback Method

dvisc	0.0004954	Pa×s	547.31	Joback Method
dvisc	0.0003440	Pa×s	601.80	Joback Method
dvisc	0.0002538	Pa×s	656.29	Joback Method
dvisc	0.0001961	Pa×s	710.77	Joback Method
dvisc	0.0001573	Pa×s	765.26	Joback Method
dvisc	0.0001299	Pa×s	819.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22359677&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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