NABUMETONE

Other names: 2-Butanone, 4-(6-methoxy-2-naphthalenyl)-
4-(6-Methoxy-2-naphthalenyl)-2-butanone
4-(6-Methoxy-2-naphthyl)-2-butanone
4-(6-Methoxy-2-naphyl)-2-butanone
4-(6-methoxynaphthalen-2-yl)butan-2-one
Arthaxan
BRL 147777
BRL-14777
Balmox
Consolan
Nabumeton
Nabuser
Relafen
Relifen
Relifex

Inchi: InChI=1S/C15H16O2/c1-11(16)3-4-12-5-6-14-10-15(17-2)8-7-13(14)9-12/h5-10H,3-4H2,

InchiKey: BLXXJMDCKKHMKV-UHFFFAOYSA-N

Formula: C15H16O2

SMILES: COc1ccc2cc(CCC(C)=O)ccc2c1

Mol. weight [g/mol]: 228.29

Physical Properties

Property code	Value	Unit	Source
hfus	27.68	kJ/mol	Joback Method
ie	7.67	eV	Cheméo Relay (1.0)
log10ws	-1.46		Aqueous Solubility Prediction Method
logp	3.370		Crippen Method
mcvol	186.430	ml/mol	McGowan Method
tb	642.82	K	Cheméo Relay (1.0)
tf	349.51	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.00	J/mol×K	674.51	Joback Method
cpg	498.93	J/mol×K	711.66	Joback Method
cpg	512.88	J/mol×K	748.81	Joback Method
cpg	525.90	J/mol×K	785.95	Joback Method
cpg	538.04	J/mol×K	823.10	Joback Method
cpg	549.35	J/mol×K	860.25	Joback Method
cpg	559.88	J/mol×K	897.40	Joback Method
dvisc	0.0011670	Pa×s	415.13	Joback Method
dvisc	0.0007887	Pa×s	458.36	Joback Method
dvisc	0.0005703	Pa×s	501.59	Joback Method
dvisc	0.0004341	Pa×s	544.82	Joback Method
dvisc	0.0003440	Pa×s	588.05	Joback Method
dvisc	0.0002814	Pa×s	631.28	Joback Method
dvisc	0.0002362	Pa×s	674.51	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42924538&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point