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

CAS: 42924-53-8

Physical Properties

Property code	Value	Unit	Source
gf	41.30	kJ/mol	Joback Method
hf	-193.07	kJ/mol	Joback Method
hfus	27.68	kJ/mol	Joback Method
hvap	63.38	kJ/mol	Joback Method
log10ws	-1.46		Aqueous Solubility Prediction Method
logp	3.370		Crippen Method
mcvol	186.430	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	2103.00		NIST Webbook
tb	674.51	K	Joback Method
tc	897.40	K	Joback Method
tf	415.13	K	Joback Method

vc	0.714	m3/kmol	Joback Method

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42924538&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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