Naproxen methyl ester

Other names:	(+)-Naproxen methyl ester
	2-Naphthaleneacetic acid, 6-methoxy-«alpha»-methyl-, methyl ester, (+)-
	2-Naphthaleneacetic acid, 6-methoxy-Â«alphaÂ»-methyl-, methyl ester, (+)-
	Methyl 2-(6-methoxy-2-naphthyl)propanoate, (S)-
	Naproxen, methyl deriv.
	Naproxen, methylated
	methyl 2-(6-methoxynaphthalen-2-yl)propanoate
Inchi:	InChI=1S/C15H16O3/c1-10(15(16)18-3)11-4-5-13-9-14(17-2)7-6-12(13)8-11/h4-10H,1-3H
InchiKey:	ZFYFBPCRUQZGJE-UHFFFAOYSA-N
Formula:	C15H16O3
SMILES:	COC(=O)C(C)c1ccc2cc(OC)ccc2c1
Mol. weight [g/mol]:	244.29
CAS:	26159-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-66.14	kJ/mol	Joback Method
hf	-330.57	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	65.40	kJ/mol	Joback Method
log10ws	-4.78		Aqueous Solubility Prediction Method
logp	3.125		Crippen Method
mcvol	192.300	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	340.30		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	340.30		NIST Webbook
tb	696.49	K	Joback Method
tc	920.81	K	Joback Method
tf	422.36	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.49	J/mol×K	696.49	Joback Method
cpg	525.37	J/mol×K	733.88	Joback Method
cpg	539.25	J/mol×K	771.26	Joback Method
cpg	552.17	J/mol×K	808.65	Joback Method
cpg	564.15	J/mol×K	846.04	Joback Method
cpg	575.23	J/mol×K	883.42	Joback Method
cpg	585.44	J/mol×K	920.81	Joback Method
dvisc	0.0010097	Pa×s	422.36	Joback Method
dvisc	0.0006532	Pa×s	468.05	Joback Method
dvisc	0.0004566	Pa×s	513.74	Joback Method
dvisc	0.0003384	Pa×s	559.42	Joback Method
dvisc	0.0002624	Pa×s	605.11	Joback Method
dvisc	0.0002109	Pa×s	650.80	Joback Method
dvisc	0.0001744	Pa×s	696.49	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26159353&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume