

1-Naphthaleneacetic acid, dodecyl ester

Inchi:	InChI=1S/C24H34O2/c1-2-3-4-5-6-7-8-9-10-13-19-26-24(25)20-22-17-14-16-21-15-11-12
InchiKey:	RCDIZPLHRKGGGM-UHFFFAOYSA-N
Formula:	C24H34O2
SMILES:	CCCCCCCCCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]:	354.53

Physical Properties

Property code	Value	Unit	Source
gf	126.71	kJ/mol	Joback Method
hf	-367.36	kJ/mol	Joback Method
hfus	51.37	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-7.96		Crippen Method
logp	6.846		Crippen Method
mvol	313.240	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	875.45	K	Joback Method
tc	1081.71	K	Joback Method
tf	504.04	K	Joback Method
vc	1.218	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.80	J/molxK	875.45	Joback Method
cpg	1011.41	J/molxK	909.83	Joback Method
cpg	1027.95	J/molxK	944.20	Joback Method
cpg	1043.48	J/molxK	978.58	Joback Method
cpg	1058.08	J/molxK	1012.95	Joback Method
cpg	1071.81	J/molxK	1047.33	Joback Method
cpg	1084.76	J/molxK	1081.71	Joback Method
dvisc	0.0007865	Paxs	504.04	Joback Method

dvisc	0.0004451	Paxs	565.94	Joback Method
dvisc	0.0002818	Paxs	627.84	Joback Method
dvisc	0.0001937	Paxs	689.75	Joback Method
dvisc	0.0001416	Paxs	751.65	Joback Method
dvisc	0.0001086	Paxs	813.55	Joback Method
dvisc	0.0000865	Paxs	875.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U415035&Units=SI

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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