

1-Naphthaleneacetic acid, tetradecyl ester

Inchi:	InChI=1S/C26H38O2/c1-2-3-4-5-6-7-8-9-10-11-12-15-21-28-26(27)22-24-19-16-18-23-17
InchiKey:	YKGAHAJPZRZENW-UHFFFAOYSA-N
Formula:	C26H38O2
SMILES:	CCCCCCCCCCCCCOC(=O)Cc1cccc2cccc12
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	143.55	kJ/mol	Joback Method
hf	-408.64	kJ/mol	Joback Method
hfus	56.55	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	7.627		Crippen Method
mcvol	341.420	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	1896.00		NIST Webbook
tb	921.21	K	Joback Method
tc	1131.10	K	Joback Method
tf	526.58	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.49	J/molxK	921.21	Joback Method
cpg	1134.67	J/molxK	956.19	Joback Method
cpg	1151.73	J/molxK	991.17	Joback Method
cpg	1167.75	J/molxK	1026.16	Joback Method
cpg	1182.83	J/molxK	1061.14	Joback Method
cpg	1197.03	J/molxK	1096.12	Joback Method
cpg	1210.45	J/molxK	1131.10	Joback Method
dvisc	0.0006524	Paxs	526.58	Joback Method
dvisc	0.0003606	Paxs	592.35	Joback Method

dvisc	0.0002244	Paxs	658.12	Joback Method
dvisc	0.0001522	Paxs	723.89	Joback Method
dvisc	0.0001101	Paxs	789.67	Joback Method
dvisc	0.0000838	Paxs	855.44	Joback Method
dvisc	0.0000662	Paxs	921.21	Joback Method

Sources

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=U415037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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