

1-Naphthaleneacetic acid, tridec-2-yn-1-yl ester

Inchi:	InChI=1S/C25H32O2/c1-2-3-4-5-6-7-8-9-10-11-14-20-27-25(26)21-23-18-15-17-22-16-12
InchiKey:	RROHAZYDKAJJDE-UHFFFAOYSA-N
Formula:	C25H32O2
SMILES:	CCCCCCCCC#CCOC(=O)Cc1cccc2cccc12
Mol. weight [g/mol]:	364.52

Physical Properties

Property code	Value	Unit	Source
gf	337.93	kJ/mol	Joback Method
hf	-115.70	kJ/mol	Joback Method
hfus	57.09	kJ/mol	Joback Method
hvap	87.13	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	6.460		Crippen Method
mvol	318.730	ml/mol	McGowan Method
pc	1230.28	kPa	Joback Method
rinpol	1565.00		NIST Webbook
rinpol	1565.00		NIST Webbook
tb	907.33	K	Joback Method
tc	1124.99	K	Joback Method
tf	621.41	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.36	J/mol×K	907.33	Joback Method
cpg	1018.55	J/mol×K	943.61	Joback Method
cpg	1034.66	J/mol×K	979.88	Joback Method
cpg	1049.76	J/mol×K	1016.16	Joback Method
cpg	1063.93	J/mol×K	1052.44	Joback Method
cpg	1077.25	J/mol×K	1088.71	Joback Method
cpg	1089.82	J/mol×K	1124.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415056&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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