

1-Naphthaleneacetic acid, 8-chlorooctyl ester

Inchi:	InChI=1S/C20H25ClO2/c21-14-7-3-1-2-4-8-15-23-20(22)16-18-12-9-11-17-10-5-6-13-19
InchiKey:	IIAVWHJSSYHUCD-UHFFFAOYSA-N
Formula:	C20H25ClO2
SMILES:	O=C(Cc1cccc2cccc12)OCCCCCCCCCl
Mol. weight [g/mol]:	332.86

Physical Properties

Property code	Value	Unit	Source
gf	81.10	kJ/mol	Joback Method
hf	-300.54	kJ/mol	Joback Method
hfus	45.21	kJ/mol	Joback Method
hvap	78.23	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.505		Crippen Method
mvol	269.120	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
tb	821.36	K	Joback Method
tc	1032.82	K	Joback Method
tf	488.88	K	Joback Method
vc	1.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.37	J/mol×K	821.36	Joback Method
cpg	800.93	J/mol×K	856.60	Joback Method
cpg	815.48	J/mol×K	891.85	Joback Method
cpg	829.10	J/mol×K	927.09	Joback Method
cpg	841.85	J/mol×K	962.34	Joback Method
cpg	853.80	J/mol×K	997.58	Joback Method
cpg	865.00	J/mol×K	1032.82	Joback Method
dvisc	0.0009419	Paxs	488.88	Joback Method

dvisc	0.0005693	Paxs	544.29	Joback Method
dvisc	0.0003777	Paxs	599.71	Joback Method
dvisc	0.0002685	Paxs	655.12	Joback Method
dvisc	0.0002014	Paxs	710.53	Joback Method
dvisc	0.0001574	Paxs	765.95	Joback Method
dvisc	0.0001272	Paxs	821.36	Joback Method

Sources

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=U415054&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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