

Phenylacetic acid, 2-naphthyl ester

Inchi:	InChI=1S/C18H14O2/c19-18(12-14-6-2-1-3-7-14)20-17-11-10-15-8-4-5-9-16(15)13-17/h1
InchiKey:	GOALADUJAUJGWAQ-UHFFFAOYSA-N
Formula:	C18H14O2
SMILES:	O=C(Cc1ccccc1)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	262.30

Physical Properties

Property code	Value	Unit	Source
gf	188.60	kJ/mol	Joback Method
hf	-6.99	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	71.67	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.988		Crippen Method
mcvol	204.940	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook
tb	764.85	K	Joback Method
tc	1016.15	K	Joback Method
tf	462.84	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.38	J/molxK	764.85	Joback Method
cpg	571.16	J/molxK	806.73	Joback Method
cpg	584.66	J/molxK	848.62	Joback Method
cpg	597.01	J/molxK	890.50	Joback Method
cpg	608.31	J/molxK	932.38	Joback Method
cpg	618.67	J/molxK	974.26	Joback Method
cpg	628.19	J/molxK	1016.15	Joback Method
dvisc	0.0010869	Paxs	462.84	Joback Method

dvisc	0.0006978	Paxs	513.18	Joback Method
dvisc	0.0004848	Paxs	563.51	Joback Method
dvisc	0.0003576	Paxs	613.85	Joback Method
dvisc	0.0002762	Paxs	664.18	Joback Method
dvisc	0.0002213	Paxs	714.52	Joback Method
dvisc	0.0001825	Paxs	764.85	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=U307537&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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