

3-Phenylpropionic acid, 2- naphthyl ester

Inchi:	InChI=1S/C19H16O2/c20-19(13-10-15-6-2-1-3-7-15)21-18-12-11-16-8-4-5-9-17(16)14-18
InchiKey:	UJLMWHLDDQYNCQZ-UHFFFAOYSA-N
Formula:	C19H16O2
SMILES:	O=C(CCc1ccccc1)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	276.33

Physical Properties

Property code	Value	Unit	Source
gf	197.02	kJ/mol	Joback Method
hf	-27.63	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.378		Crippen Method
mcvol	219.030	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinsol	2420.00		NIST Webbook
tb	787.73	K	Joback Method
tc	1033.89	K	Joback Method
tf	474.11	K	Joback Method
vc	0.830	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.60	J/molxK	787.73	Joback Method
cpg	674.43	J/molxK	992.86	Joback Method
cpg	663.72	J/molxK	951.84	Joback Method
cpg	652.10	J/molxK	910.81	Joback Method
cpg	639.44	J/molxK	869.78	Joback Method
cpg	625.64	J/molxK	828.76	Joback Method
cpg	684.31	J/molxK	1033.89	Joback Method
dvisc	0.0001640	Paxs	787.73	Joback Method
dvisc	0.0001998	Paxs	735.46	Joback Method

dvisc	0.0002508	Paxs	683.19	Joback Method
dvisc	0.0003269	Paxs	630.92	Joback Method
dvisc	0.0004470	Paxs	578.65	Joback Method
dvisc	0.0006504	Paxs	526.38	Joback Method
dvisc	0.0010280	Paxs	474.11	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=U307787&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

Latest version available from:

<https://www.chemeo.com/cid/56-074-8/3-Phenylpropionic-acid-2-naphthyl-ester.pdf>

Generated by Cheméo on 2024-04-29 14:54:27.847117021 +0000 UTC m=+16691716.767694333.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.