

Pimelic acid, 2-naphthyl propyl ester

Inchi:	InChI=1S/C20H24O4/c1-2-14-23-19(21)10-4-3-5-11-20(22)24-18-13-12-16-8-6-7-9-17(16)
InchiKey:	MQDIDYTZRBNXNGZ-UHFFFAOYSA-N
Formula:	C20H24O4
SMILES:	CCCOC(=O)CCCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	328.40

Physical Properties

Property code	Value	Unit	Source
gf	-140.89	kJ/mol	Joback Method
hf	-529.60	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.649		Crippen Method
mvol	264.320	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	2679.00		NIST Webbook
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tb	860.22	K	Joback Method
tc	1074.09	K	Joback Method
tf	531.12	K	Joback Method
vc	1.018	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.86	J/molxK	860.22	Joback Method
cpg	817.37	J/molxK	895.87	Joback Method
cpg	830.81	J/molxK	931.51	Joback Method
cpg	843.24	J/molxK	967.16	Joback Method
cpg	854.70	J/molxK	1002.80	Joback Method
cpg	865.25	J/molxK	1038.45	Joback Method
cpg	874.92	J/molxK	1074.09	Joback Method
dvisc	0.0007126	Paxs	531.12	Joback Method

dvisc	0.0004495	Paxs	585.97	Joback Method
dvisc	0.0003068	Paxs	640.82	Joback Method
dvisc	0.0002224	Paxs	695.67	Joback Method
dvisc	0.0001690	Paxs	750.52	Joback Method
dvisc	0.0001333	Paxs	805.37	Joback Method
dvisc	0.0001084	Paxs	860.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416707&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

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
log_p:	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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