

Pimelic acid, 2-naphthyl octyl ester

Inchi:	InChI=1S/C25H34O4/c1-2-3-4-5-6-12-19-28-24(26)15-8-7-9-16-25(27)29-23-18-17-21-13
InchiKey:	ULLSUBIYIXQOKR-UHFFFAOYSA-N
Formula:	C25H34O4
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	398.54

Physical Properties

Property code	Value	Unit	Source
gf	-98.79	kJ/mol	Joback Method
hf	-632.80	kJ/mol	Joback Method
hfus	56.75	kJ/mol	Joback Method
hvap	94.13	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.599		Crippen Method
mvol	334.770	ml/mol	McGowan Method
pc	1137.50	kPa	Joback Method
rinpol	3183.00		NIST Webbook
rinpol	3183.00		NIST Webbook
tb	974.62	K	Joback Method
tc	1194.68	K	Joback Method
tf	587.47	K	Joback Method
vc	1.298	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1100.84	J/molxK	974.62	Joback Method
cpg	1116.48	J/molxK	1011.30	Joback Method
cpg	1130.91	J/molxK	1047.97	Joback Method
cpg	1144.21	J/molxK	1084.65	Joback Method
cpg	1156.45	J/molxK	1121.33	Joback Method
cpg	1167.69	J/molxK	1158.00	Joback Method
cpg	1178.00	J/molxK	1194.68	Joback Method
dvisc	0.0004444	Paxs	587.47	Joback Method

dvisc	0.0002642	Paxs	652.00	Joback Method
dvisc	0.0001726	Paxs	716.52	Joback Method
dvisc	0.0001209	Paxs	781.05	Joback Method
dvisc	0.0000894	Paxs	845.57	Joback Method
dvisc	0.0000690	Paxs	910.10	Joback Method
dvisc	0.0000552	Paxs	974.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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