

Pimelic acid, hexyl 3-phenylpropyl ester

Inchi:	InChI=1S/C22H34O4/c1-2-3-4-11-18-25-21(23)16-9-6-10-17-22(24)26-19-12-15-20-13-7
InchiKey:	FFLINFZTVXTQRR-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	362.50

Physical Properties

Property code	Value	Unit	Source
gf	-221.07	kJ/mol	Joback Method
hf	-750.48	kJ/mol	Joback Method
hfus	52.35	kJ/mol	Joback Method
hvap	85.15	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.236		Crippen Method
mvol	311.960	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2783.00		NIST Webbook
rinpol	2783.00		NIST Webbook
tb	882.02	K	Joback Method
tc	1084.27	K	Joback Method
tf	508.44	K	Joback Method
vc	1.208	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.85	J/molxK	882.02	Joback Method
cpg	1069.21	J/molxK	1050.57	Joback Method
cpg	1057.25	J/molxK	1016.86	Joback Method
cpg	1044.16	J/molxK	983.15	Joback Method
cpg	1029.92	J/molxK	949.44	Joback Method
cpg	1014.49	J/molxK	915.73	Joback Method
cpg	1080.10	J/molxK	1084.27	Joback Method
dvisc	0.0000406	Paxs	882.02	Joback Method

dvisc	0.0000533	Paxs	819.76	Joback Method
dvisc	0.0000731	Paxs	757.49	Joback Method
dvisc	0.0001061	Paxs	695.23	Joback Method
dvisc	0.0001657	Paxs	632.97	Joback Method
dvisc	0.0002853	Paxs	570.70	Joback Method
dvisc	0.0005610	Paxs	508.44	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=U416513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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