Pimelic acid, heptyl phenethyl ester

Inchi: InChI=1S/C22H34O4/c1-2-3-4-5-12-18-25-21(23)15-10-7-11-16-22(24)26-19-17-20-13-8
InchiKey: GUZCKECTMCPFPA-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCCCCCCOC(=O)CCCCCC(=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
mcvol	311.960	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	882.02	K	Joback Method
tc	1084.27	K	Joback Method
tf	508.44	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.85	J/mol×K	882.02	Joback Method
cpg	1014.49	J/mol×K	915.73	Joback Method
cpg	1029.92	J/mol×K	949.44	Joback Method
cpg	1044.16	J/mol×K	983.15	Joback Method
cpg	1057.25	J/mol×K	1016.86	Joback Method
cpg	1069.21	J/mol×K	1050.57	Joback Method
cpg	1080.10	J/mol×K	1084.27	Joback Method
dvisc	0.0005610	Pa×s	508.44	Joback Method

dvisc	0.0002853	Pa×s	570.70	Joback Method
dvisc	0.0001657	Pa×s	632.97	Joback Method
dvisc	0.0001061	Pa×s	695.23	Joback Method
dvisc	0.0000731	Pa×s	757.49	Joback Method
dvisc	0.0000533	Pa×s	819.76	Joback Method
dvisc	0.0000406	Pa×s	882.02	Joback Method

Sources

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=U416500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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