Pimelic acid, octyl phenethyl ester

Inchi: InChI=1S/C23H36O4/c1-2-3-4-5-6-13-19-26-22(24)16-11-8-12-17-23(25)27-20-18-21-14
InchiKey: NJTGYRWKSDSZFL-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCCCCOC(=O)CCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-212.65	kJ/mol	Joback Method
hf	-771.12	kJ/mol	Joback Method
hfus	54.94	kJ/mol	Joback Method
hvap	87.38	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.627		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1108.89	kPa	Joback Method
rinpol	2973.00		NIST Webbook
rinpol	2973.00		NIST Webbook
tb	904.90	K	Joback Method
tc	1109.91	K	Joback Method
tf	519.71	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.61	J/mol×K	904.90	Joback Method
cpg	1075.49	J/mol×K	939.07	Joback Method
cpg	1091.08	J/mol×K	973.24	Joback Method
cpg	1105.44	J/mol×K	1007.40	Joback Method
cpg	1118.60	J/mol×K	1041.57	Joback Method
cpg	1130.59	J/mol×K	1075.74	Joback Method
cpg	1141.46	J/mol×K	1109.91	Joback Method
dvisc	0.0005005	Pa×s	519.71	Joback Method

dvisc	0.0002518	Pa×s	583.91	Joback Method
dvisc	0.0001452	Pa×s	648.11	Joback Method
dvisc	0.0000925	Pa×s	712.30	Joback Method
dvisc	0.0000634	Pa×s	776.50	Joback Method
dvisc	0.0000461	Pa×s	840.70	Joback Method
dvisc	0.0000350	Pa×s	904.90	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=U416501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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