Pimelic acid, di(phenethyl) ester

Inchi: InChI=1S/C23H28O4/c24-22(26-18-16-20-10-4-1-5-11-20)14-8-3-9-15-23(25)27-19-17-2
InchiKey: LSKMSPAJKQIPCN-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: O=C(CCCCCC(=O)OCCc1ccccc1)OCCc1ccccc1
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-100.24	kJ/mol	Joback Method
hf	-534.59	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	89.66	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.509		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1400.64	kPa	Joback Method
rinpol	2284.00		NIST Webbook
rinpol	2284.00		NIST Webbook
tb	931.58	K	Joback Method
tc	1152.51	K	Joback Method
tf	546.13	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.01	J/mol×K	931.58	Joback Method
cpg	972.52	J/mol×K	968.40	Joback Method
cpg	985.70	J/mol×K	1005.22	Joback Method
cpg	997.60	J/mol×K	1042.04	Joback Method
cpg	1008.29	J/mol×K	1078.87	Joback Method
cpg	1017.81	J/mol×K	1115.69	Joback Method
cpg	1026.22	J/mol×K	1152.51	Joback Method
dvisc	0.0004322	Pa×s	546.13	Joback Method

dvisc	0.0002297	Pa×s	610.37	Joback Method
dvisc	0.0001377	Pa×s	674.61	Joback Method
dvisc	0.0000902	Pa×s	738.86	Joback Method
dvisc	0.0000633	Pa×s	803.10	Joback Method
dvisc	0.0000468	Pa×s	867.34	Joback Method
dvisc	0.0000360	Pa×s	931.58	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416506&Units=SI

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