Pimelic acid, decyl 4-formylphenyl ester

Inchi: InChI=1S/C24H36O5/c1-2-3-4-5-6-7-8-12-19-28-23(26)13-10-9-11-14-24(27)29-22-17-15
InchiKey: SNEPPHRVYYUQCJ-UHFFFAOYSA-N
Formula: C24H36O5
SMILES: CCCCCCCCCCOC(=O)CCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-313.38	kJ/mol	Joback Method
hf	-888.81	kJ/mol	Joback Method
hfus	59.43	kJ/mol	Joback Method
hvap	96.99	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.039		Crippen Method
mcvol	341.710	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	3233.00		NIST Webbook
rinpol	3233.00		NIST Webbook
tb	981.42	K	Joback Method
tc	1201.57	K	Joback Method
tf	585.50	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.88	J/mol×K	981.42	Joback Method
cpg	1195.90	J/mol×K	1164.88	Joback Method
cpg	1186.21	J/mol×K	1128.19	Joback Method
cpg	1175.21	J/mol×K	1091.50	Joback Method
cpg	1162.85	J/mol×K	1054.80	Joback Method
cpg	1149.09	J/mol×K	1018.11	Joback Method
cpg	1204.32	J/mol×K	1201.57	Joback Method
dvisc	0.0000328	Pa×s	981.42	Joback Method

dvisc	0.0000423	Pa×s	915.43	Joback Method
dvisc	0.0000569	Pa×s	849.45	Joback Method
dvisc	0.0000803	Pa×s	783.46	Joback Method
dvisc	0.0001209	Pa×s	717.47	Joback Method
dvisc	0.0001976	Pa×s	651.49	Joback Method
dvisc	0.0003609	Pa×s	585.50	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=U416651&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