Pimelic acid, 4-formylphenyl hexyl ester

Inchi: InChI=1S/C20H28O5/c1-2-3-4-8-15-24-19(22)9-6-5-7-10-20(23)25-18-13-11-17(16-21)12
InchiKey: FTRXKOQQOBPAQN-UHFFFAOYSA-N
Formula: C20H28O5
SMILES: CCCCCCOC(=O)CCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 348.43

Physical Properties

Property code	Value	Unit	Source
gf	-347.06	kJ/mol	Joback Method
hf	-806.25	kJ/mol	Joback Method
hfus	49.07	kJ/mol	Joback Method
hvap	88.08	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.478		Crippen Method
mcvol	285.350	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	2804.00		NIST Webbook
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tb	889.90	K	Joback Method
tc	1096.16	K	Joback Method
tf	540.42	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.64	J/mol×K	889.90	Joback Method
cpg	907.95	J/mol×K	924.28	Joback Method
cpg	921.09	J/mol×K	958.65	Joback Method
cpg	933.10	J/mol×K	993.03	Joback Method
cpg	944.00	J/mol×K	1027.40	Joback Method
cpg	953.80	J/mol×K	1061.78	Joback Method
cpg	962.54	J/mol×K	1096.16	Joback Method
dvisc	0.0005637	Pa×s	540.42	Joback Method

dvisc	0.0003223	Pa×s	598.67	Joback Method
dvisc	0.0002035	Pa×s	656.91	Joback Method
dvisc	0.0001385	Pa×s	715.16	Joback Method
dvisc	0.0000998	Pa×s	773.41	Joback Method
dvisc	0.0000754	Pa×s	831.65	Joback Method
dvisc	0.0000590	Pa×s	889.90	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=U416648&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