

Pimelic acid, 4-formylphenyl heptyl ester

Inchi:	InChI=1S/C21H30O5/c1-2-3-4-5-9-16-25-20(23)10-7-6-8-11-21(24)26-19-14-12-18(17-22)
InchiKey:	PSBYLABTXBDZHP-UHFFFAOYSA-N
Formula:	C21H30O5
SMILES:	CCCCCCCOC(=O)CCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]:	362.46

Physical Properties

Property code	Value	Unit	Source
gf	-338.64	kJ/mol	Joback Method
hf	-826.89	kJ/mol	Joback Method
hfus	51.66	kJ/mol	Joback Method
hvap	90.31	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.869		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	2905.00		NIST Webbook
tb	912.78	K	Joback Method
tc	1121.15	K	Joback Method
tf	551.69	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.82	J/molxK	912.78	Joback Method
cpg	1013.53	J/molxK	1086.42	Joback Method
cpg	1003.71	J/molxK	1051.70	Joback Method
cpg	992.76	J/molxK	1016.97	Joback Method
cpg	980.65	J/molxK	982.24	Joback Method
cpg	967.35	J/molxK	947.51	Joback Method
cpg	1022.23	J/molxK	1121.15	Joback Method
dvisc	0.0000511	Paxs	912.78	Joback Method
dvisc	0.0000655	Paxs	852.60	Joback Method

dvisc	0.0000871	Paxs	792.42	Joback Method
dvisc	0.0001213	Paxs	732.23	Joback Method
dvisc	0.0001794	Paxs	672.05	Joback Method
dvisc	0.0002865	Paxs	611.87	Joback Method
dvisc	0.0005069	Paxs	551.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U416649&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

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