

Pimelic acid, 4-chloro-3-methylphenyl heptyl ester

Inchi:	InChI=1S/C21H31ClO4/c1-3-4-5-6-10-15-25-20(23)11-8-7-9-12-21(24)26-18-13-14-19(2)
InchiKey:	JDDZIAPEKCYALM-UHFFFAOYSA-N
Formula:	C21H31ClO4
SMILES:	CCCCCCCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	382.92

Physical Properties

Property code	Value	Unit	Source
gf	-260.68	kJ/mol	Joback Method
hf	-768.52	kJ/mol	Joback Method
hfus	53.18	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	6.018		Crippen Method
mvol	310.110	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinpol	2869.00		NIST Webbook
rinpol	2869.00		NIST Webbook
tb	906.53	K	Joback Method
tc	1114.56	K	Joback Method
tf	552.13	K	Joback Method
vc	1.200	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.52	J/molxK	906.53	Joback Method
cpg	978.62	J/molxK	941.20	Joback Method
cpg	992.49	J/molxK	975.87	Joback Method
cpg	1005.17	J/molxK	1010.55	Joback Method
cpg	1016.69	J/molxK	1045.22	Joback Method
cpg	1027.05	J/molxK	1079.89	Joback Method
cpg	1036.30	J/molxK	1114.56	Joback Method
dvisc	0.0003804	Paxs	552.13	Joback Method

dvisc	0.0002201	Paxs	611.20	Joback Method
dvisc	0.0001402	Paxs	670.26	Joback Method
dvisc	0.0000961	Paxs	729.33	Joback Method
dvisc	0.0000697	Paxs	788.40	Joback Method
dvisc	0.0000529	Paxs	847.46	Joback Method
dvisc	0.0000416	Paxs	906.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416687&Units=SI
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

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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