

Pimelic acid, 3-chlorophenyl octyl ester

Inchi:	InChI=1S/C21H31ClO4/c1-2-3-4-5-6-10-16-25-20(23)14-8-7-9-15-21(24)26-19-13-11-12
InchiKey:	NTVPYDZLHFAXMP-UHFFFAOYSA-N
Formula:	C21H31ClO4
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	382.92

Physical Properties

Property code	Value	Unit	Source
gf	-251.05	kJ/mol	Joback Method
hf	-757.05	kJ/mol	Joback Method
hfus	53.57	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	6.100		Crippen Method
mvol	310.110	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2962.00		NIST Webbook
rinpol	2962.00		NIST Webbook
tb	901.55	K	Joback Method
tc	1108.65	K	Joback Method
tf	539.61	K	Joback Method
vc	1.200	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.34	J/molxK	901.55	Joback Method
cpg	1028.51	J/molxK	1074.14	Joback Method
cpg	1017.96	J/molxK	1039.62	Joback Method
cpg	1006.30	J/molxK	1005.10	Joback Method
cpg	993.50	J/molxK	970.58	Joback Method
cpg	979.52	J/molxK	936.07	Joback Method
cpg	1037.97	J/molxK	1108.65	Joback Method
dvisc	0.0000408	Paxs	901.55	Joback Method

dvisc	0.0000526	Paxs	841.23	Joback Method
dvisc	0.0000704	Paxs	780.90	Joback Method
dvisc	0.0000989	Paxs	720.58	Joback Method
dvisc	0.0001480	Paxs	660.26	Joback Method
dvisc	0.0002402	Paxs	599.93	Joback Method
dvisc	0.0004342	Paxs	539.61	Joback Method

Sources

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=U416675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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