

Pimelic acid, 4-chlorobenzyl pentyl ester

Inchi:	InChI=1S/C19H27ClO4/c1-2-3-7-14-23-18(21)8-5-4-6-9-19(22)24-15-16-10-12-17(20)13
InchiKey:	MYNJRNQFQCYYCK-UHFFFAOYSA-N
Formula:	C19H27ClO4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	354.87

Physical Properties

Property code	Value	Unit	Source
gf	-267.89	kJ/mol	Joback Method
hf	-715.77	kJ/mol	Joback Method
hfus	48.39	kJ/mol	Joback Method
hvap	83.52	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.067		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2559.00		NIST Webbook
rinpol	2559.00		NIST Webbook
tb	855.79	K	Joback Method
tc	1060.17	K	Joback Method
tf	517.07	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.29	J/molxK	855.79	Joback Method
cpg	861.04	J/molxK	889.85	Joback Method
cpg	874.69	J/molxK	923.92	Joback Method
cpg	887.26	J/molxK	957.98	Joback Method
cpg	898.76	J/molxK	992.04	Joback Method
cpg	909.23	J/molxK	1026.10	Joback Method
cpg	918.69	J/molxK	1060.17	Joback Method
dvisc	0.0005380	Paxs	517.07	Joback Method

dvisc	0.0003045	Paxs	573.52	Joback Method
dvisc	0.0001909	Paxs	629.98	Joback Method
dvisc	0.0001292	Paxs	686.43	Joback Method
dvisc	0.0000928	Paxs	742.88	Joback Method
dvisc	0.0000698	Paxs	799.34	Joback Method
dvisc	0.0000546	Paxs	855.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from:

<https://www.cheméo.com/cid/99-905-8/Pimelic-acid-4-chlorobenzyl-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-19 20:43:58.035979362 +0000 UTC m=+15848686.956556679.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.