

Sebacic acid, 4-chloro-3-methylphenyl hexyl ester

Inchi:	InChI=1S/C23H35ClO4/c1-3-4-5-12-17-27-22(25)13-10-8-6-7-9-11-14-23(26)28-20-15-16
InchiKey:	OQWAANCAAKHXAV-UHFFFAOYSA-N
Formula:	C23H35ClO4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	410.98

Physical Properties

Property code	Value	Unit	Source
gf	-243.84	kJ/mol	Joback Method
hf	-809.80	kJ/mol	Joback Method
hfus	58.36	kJ/mol	Joback Method
hvap	93.09	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.798		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1061.02	kPa	Joback Method
rinpola	3082.00		NIST Webbook
tb	952.29	K	Joback Method
tc	1166.50	K	Joback Method
tf	574.67	K	Joback Method
vc	1.312	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.19	J/molxK	952.29	Joback Method
cpg	1099.71	J/molxK	987.99	Joback Method
cpg	1113.87	J/molxK	1023.69	Joback Method
cpg	1126.72	J/molxK	1059.39	Joback Method
cpg	1138.27	J/molxK	1095.10	Joback Method
cpg	1148.57	J/molxK	1130.80	Joback Method
cpg	1157.64	J/molxK	1166.50	Joback Method
dvisc	0.0003047	Paxs	574.67	Joback Method
dvisc	0.0001724	Paxs	637.61	Joback Method

dvisc	0.0001081	Paxs	700.54	Joback Method
dvisc	0.0000732	Paxs	763.48	Joback Method
dvisc	0.0000526	Paxs	826.42	Joback Method
dvisc	0.0000396	Paxs	889.35	Joback Method
dvisc	0.0000309	Paxs	952.29	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=U354848&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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