

Sebacic acid, 3-chlorophenyl heptyl ester

Inchi:	InChI=1S/C23H35ClO4/c1-2-3-4-9-12-18-27-22(25)16-10-7-5-6-8-11-17-23(26)28-21-15
InchiKey:	QESASWSHBURXED-UHFFFAOYSA-N
Formula:	C23H35ClO4
SMILES:	CCCCCCCC(=O)CCCCCCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	410.98

Physical Properties

Property code	Value	Unit	Source
gf	-234.21	kJ/mol	Joback Method
hf	-798.33	kJ/mol	Joback Method
hfus	58.75	kJ/mol	Joback Method
hvap	92.43	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	6.880		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	3068.00		NIST Webbook
tb	947.31	K	Joback Method
tc	1160.48	K	Joback Method
tf	562.15	K	Joback Method
vc	1.312	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.97	J/molxK	947.31	Joback Method
cpg	1100.59	J/molxK	982.84	Joback Method
cpg	1114.89	J/molxK	1018.37	Joback Method
cpg	1127.90	J/molxK	1053.89	Joback Method
cpg	1139.65	J/molxK	1089.42	Joback Method
cpg	1150.19	J/molxK	1124.95	Joback Method
cpg	1159.55	J/molxK	1160.48	Joback Method
dvisc	0.0003455	Paxs	562.15	Joback Method
dvisc	0.0001870	Paxs	626.34	Joback Method

dvisc	0.0001135	Paxs	690.54	Joback Method
dvisc	0.0000750	Paxs	754.73	Joback Method
dvisc	0.0000529	Paxs	818.92	Joback Method
dvisc	0.0000392	Paxs	883.12	Joback Method
dvisc	0.0000303	Paxs	947.31	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=U354863&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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