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

Inchi: InChI=1S/C24H37ClO4/c1-3-4-5-10-13-18-28-23(26)14-11-8-6-7-9-12-15-24(27)29-21-16
InchiKey: NNYMJMNJHWVVLC-UHFFFAOYSA-N
Formula: C24H37ClO4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]: 425.00

Physical Properties

Property code	Value	Unit	Source
gf	-235.42	kJ/mol	Joback Method
hf	-830.44	kJ/mol	Joback Method
hfus	60.95	kJ/mol	Joback Method
hvap	95.32	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.188		Crippen Method
mcvol	352.380	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
rinpol	3188.00		NIST Webbook
rinpol	3188.00		NIST Webbook
tb	975.17	K	Joback Method
tc	1193.89	K	Joback Method
tf	585.94	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.33	J/mol×K	975.17	Joback Method
cpg	1210.07	J/mol×K	1157.44	Joback Method
cpg	1199.85	J/mol×K	1120.98	Joback Method
cpg	1188.30	J/mol×K	1084.53	Joback Method
cpg	1175.39	J/mol×K	1048.08	Joback Method
cpg	1161.08	J/mol×K	1011.62	Joback Method
cpg	1219.02	J/mol×K	1193.89	Joback Method
dvisc	0.0000266	Pa×s	975.17	Joback Method

dvisc	0.0000341	Pa×s	910.30	Joback Method
dvisc	0.0000455	Pa×s	845.43	Joback Method
dvisc	0.0000636	Pa×s	780.56	Joback Method
dvisc	0.0000945	Pa×s	715.68	Joback Method
dvisc	0.0001520	Pa×s	650.81	Joback Method
dvisc	0.0002714	Pa×s	585.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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

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