

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

Inchi:	InChI=1S/C27H43ClO4/c1-3-4-5-6-7-10-13-16-21-31-26(29)17-14-11-8-9-12-15-18-27(30)
InchiKey:	DXUBBVSFVSRFNI-UHFFFAOYSA-N
Formula:	C27H43ClO4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	467.08

Physical Properties

Property code	Value	Unit	Source
gf	-210.16	kJ/mol	Joback Method
hf	-892.36	kJ/mol	Joback Method
hfus	68.72	kJ/mol	Joback Method
hvap	101.99	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.359		Crippen Method
mvol	394.650	ml/mol	McGowan Method
pc	838.21	kPa	Joback Method
rinpol	3500.00		NIST Webbook
tb	1043.81	K	Joback Method
tc	1282.60	K	Joback Method
tf	619.75	K	Joback Method
vc	1.536	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1331.33	J/molxK	1043.81	Joback Method
cpg	1347.88	J/molxK	1083.61	Joback Method
cpg	1362.66	J/molxK	1123.41	Joback Method
cpg	1375.73	J/molxK	1163.20	Joback Method
cpg	1387.15	J/molxK	1203.00	Joback Method
cpg	1396.99	J/molxK	1242.80	Joback Method
cpg	1405.30	J/molxK	1282.60	Joback Method
dvisc	0.0001886	Paxs	619.75	Joback Method
dvisc	0.0001025	Paxs	690.43	Joback Method

dvisc	0.0000624	Paxs	761.10	Joback Method
dvisc	0.0000413	Paxs	831.78	Joback Method
dvisc	0.0000292	Paxs	902.46	Joback Method
dvisc	0.0000217	Paxs	973.13	Joback Method
dvisc	0.0000168	Paxs	1043.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354852&Units=SI
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

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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