

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

Inchi:	InChI=1S/C26H41ClO4/c1-3-4-5-6-9-12-15-20-30-25(28)16-13-10-7-8-11-14-17-26(29)3
InchiKey:	WRRQPDAXIXTCSF-UHFFFAOYSA-N
Formula:	C26H41ClO4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	453.05

Physical Properties

Property code	Value	Unit	Source
gf	-218.58	kJ/mol	Joback Method
hf	-871.72	kJ/mol	Joback Method
hfus	66.13	kJ/mol	Joback Method
hvap	99.77	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.968		Crippen Method
mvol	380.560	ml/mol	McGowan Method
pc	886.83	kPa	Joback Method
rinpol	3398.00		NIST Webbook
rinpol	3398.00		NIST Webbook
tb	1020.93	K	Joback Method
tc	1251.86	K	Joback Method
tf	608.48	K	Joback Method
vc	1.480	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.95	J/molxK	1020.93	Joback Method
cpg	1285.21	J/molxK	1059.42	Joback Method
cpg	1299.83	J/molxK	1097.91	Joback Method
cpg	1312.85	J/molxK	1136.39	Joback Method
cpg	1324.34	J/molxK	1174.88	Joback Method
cpg	1334.34	J/molxK	1213.37	Joback Method
cpg	1342.90	J/molxK	1251.86	Joback Method
dvisc	0.0002135	Paxs	608.48	Joback Method

dvisc	0.0001172	Paxs	677.22	Joback Method
dvisc	0.0000718	Paxs	745.96	Joback Method
dvisc	0.0000478	Paxs	814.71	Joback Method
dvisc	0.0000339	Paxs	883.45	Joback Method
dvisc	0.0000253	Paxs	952.19	Joback Method
dvisc	0.0000196	Paxs	1020.93	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=U354851&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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