

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:	NNYMJMNJHWVVLG-UHFFFAOYSA-N
Formula:	C24H37ClO4
SMILES:	CCCCCCCCOC(=O)CCCCCCCC(=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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.33	J/molxK	975.17	Joback Method
cpg	1161.08	J/molxK	1011.62	Joback Method
cpg	1175.39	J/molxK	1048.08	Joback Method
cpg	1188.30	J/molxK	1084.53	Joback Method
cpg	1199.85	J/molxK	1120.98	Joback Method
cpg	1210.07	J/molxK	1157.44	Joback Method
cpg	1219.02	J/molxK	1193.89	Joback Method
dvisc	0.0002714	Paxs	585.94	Joback Method

dvisc	0.0001520	Paxs	650.81	Joback Method
dvisc	0.0000945	Paxs	715.68	Joback Method
dvisc	0.0000636	Paxs	780.56	Joback Method
dvisc	0.0000455	Paxs	845.43	Joback Method
dvisc	0.0000341	Paxs	910.30	Joback Method
dvisc	0.0000266	Paxs	975.17	Joback Method

Sources

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=U354849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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