

Sebacic acid, 4-chloro-2-methylphenyl octyl ester

Inchi:	InChI=1S/C25H39ClO4/c1-3-4-5-6-11-14-19-29-24(27)15-12-9-7-8-10-13-16-25(28)30-23
InchiKey:	QJHNGQYICWBFEO-UHFFFAOYSA-N
Formula:	C25H39ClO4
SMILES:	CCCCCCCCOC(=O)CCCCCCCC(=O)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]:	439.03

Physical Properties

Property code	Value	Unit	Source
gf	-227.00	kJ/mol	Joback Method
hf	-851.08	kJ/mol	Joback Method
hfus	63.54	kJ/mol	Joback Method
hvap	97.54	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.578		Crippen Method
mvol	366.470	ml/mol	McGowan Method
pc	939.79	kPa	Joback Method
rinpol	3206.00		NIST Webbook
rinpol	3206.00		NIST Webbook
tb	998.05	K	Joback Method
tc	1222.32	K	Joback Method
tf	597.21	K	Joback Method
vc	1.425	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.93	J/molxK	998.05	Joback Method
cpg	1222.93	J/molxK	1035.43	Joback Method
cpg	1237.39	J/molxK	1072.81	Joback Method
cpg	1250.36	J/molxK	1110.18	Joback Method
cpg	1261.89	J/molxK	1147.56	Joback Method
cpg	1272.01	J/molxK	1184.94	Joback Method
cpg	1280.79	J/molxK	1222.32	Joback Method
dvisc	0.0002411	Paxs	597.21	Joback Method

dvisc	0.0001336	Paxs	664.02	Joback Method
dvisc	0.0000825	Paxs	730.82	Joback Method
dvisc	0.0000552	Paxs	797.63	Joback Method
dvisc	0.0000393	Paxs	864.44	Joback Method
dvisc	0.0000294	Paxs	931.24	Joback Method
dvisc	0.0000229	Paxs	998.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355106&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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