

Sebacic acid, 2-chlorophenethyl decyl ester

Inchi: InChI=1S/C28H45ClO4/c1-2-3-4-5-6-9-12-17-23-32-27(30)20-13-10-7-8-11-14-21-28(31)
InchiKey: JZZFEYOPBMLGAS-UHFFFAOYSA-N
Formula: C28H45ClO4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCc1ccccc1Cl
Mol. weight [g/mol]: 481.11

Physical Properties

Property code	Value	Unit	Source
gf	-192.11	kJ/mol	Joback Method
hf	-901.53	kJ/mol	Joback Method
hfus	71.70	kJ/mol	Joback Method
hvap	103.56	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	8.230		Crippen Method
mvol	408.740	ml/mol	McGowan Method
pc	800.24	kPa	Joback Method
rinpol	3306.00		NIST Webbook
rinpol	3306.00		NIST Webbook
tb	1061.71	K	Joback Method
tc	1308.18	K	Joback Method
tf	618.50	K	Joback Method
vc	1.593	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.96	J/molxK	1061.71	Joback Method
cpg	1412.04	J/molxK	1102.79	Joback Method
cpg	1427.27	J/molxK	1143.87	Joback Method
cpg	1440.73	J/molxK	1184.94	Joback Method
cpg	1452.50	J/molxK	1226.02	Joback Method
cpg	1462.66	J/molxK	1267.10	Joback Method
cpg	1471.32	J/molxK	1308.18	Joback Method
dvisc	0.0001855	Paxs	618.50	Joback Method

dvisc	0.0000957	Paxs	692.37	Joback Method
dvisc	0.0000561	Paxs	766.24	Joback Method
dvisc	0.0000361	Paxs	840.11	Joback Method
dvisc	0.0000250	Paxs	913.97	Joback Method
dvisc	0.0000182	Paxs	987.84	Joback Method
dvisc	0.0000139	Paxs	1061.71	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=U416234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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