

Sebacic acid, 3-chlorophenethyl undecyl ester

Inchi: InChI=1S/C29H47ClO4/c1-2-3-4-5-6-7-10-13-16-23-33-28(31)20-14-11-8-9-12-15-21-29
InchiKey: HCHXPTZSZNVVIL-UHFFFAOYSA-N
Formula: C29H47ClO4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]: 495.13

Physical Properties

Property code	Value	Unit	Source
gf	-183.69	kJ/mol	Joback Method
hf	-922.17	kJ/mol	Joback Method
hfus	74.29	kJ/mol	Joback Method
hvap	105.78	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	8.620		Crippen Method
mvol	422.830	ml/mol	McGowan Method
pc	758.49	kPa	Joback Method
rinpol	3379.00		NIST Webbook
rinpol	3379.00		NIST Webbook
tb	1084.59	K	Joback Method
tc	1341.47	K	Joback Method
tf	629.77	K	Joback Method
vc	1.649	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1458.02	J/molxK	1084.59	Joback Method
cpg	1526.22	J/molxK	1298.66	Joback Method
cpg	1516.20	J/molxK	1255.85	Joback Method
cpg	1504.47	J/molxK	1213.03	Joback Method
cpg	1490.93	J/molxK	1170.22	Joback Method
cpg	1475.49	J/molxK	1127.40	Joback Method
cpg	1534.64	J/molxK	1341.47	Joback Method
dvisc	0.0000119	Paxs	1084.59	Joback Method

dvisc	0.0000156	Paxs	1008.79	Joback Method
dvisc	0.0000214	Paxs	932.98	Joback Method
dvisc	0.0000310	Paxs	857.18	Joback Method
dvisc	0.0000484	Paxs	781.38	Joback Method
dvisc	0.0000832	Paxs	705.57	Joback Method
dvisc	0.0001626	Paxs	629.77	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=U416246&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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