

Sebacic acid, 8-chlorooctyl isobutyl ester

Inchi:	InChI=1S/C22H41ClO4/c1-20(2)19-27-22(25)16-12-8-4-3-7-11-15-21(24)26-18-14-10-6-5
InchiKey:	SZXZYYKOCPREHD-UHFFFAOYSA-N
Formula:	C22H41ClO4
SMILES:	CC(C)COC(=O)CCCCCCCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]:	405.01

Physical Properties

Property code	Value	Unit	Source
gf	-347.85	kJ/mol	Joback Method
hf	-1008.03	kJ/mol	Joback Method
hfus	58.98	kJ/mol	Joback Method
hvap	86.88	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	6.429		Crippen Method
mvol	347.960	ml/mol	McGowan Method
pc	936.92	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	892.33	K	Joback Method
tc	1092.48	K	Joback Method
tf	496.94	K	Joback Method
vc	1.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.91	J/molxK	892.33	Joback Method
cpg	1202.56	J/molxK	1059.12	Joback Method
cpg	1189.26	J/molxK	1025.76	Joback Method
cpg	1174.77	J/molxK	992.40	Joback Method
cpg	1159.07	J/molxK	959.05	Joback Method
cpg	1142.13	J/molxK	925.69	Joback Method
cpg	1214.70	J/molxK	1092.48	Joback Method
dvisc	0.0000308	Paxs	892.33	Joback Method

dvisc	0.0000414	Paxs	826.43	Joback Method
dvisc	0.0000587	Paxs	760.53	Joback Method
dvisc	0.0000889	Paxs	694.63	Joback Method
dvisc	0.0001469	Paxs	628.74	Joback Method
dvisc	0.0002731	Paxs	562.84	Joback Method
dvisc	0.0005981	Paxs	496.94	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=U355529&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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