

Succinic acid, 3-methylbut-2-en-1-yl 10-chlorodecyl ester

Inchi: InChI=1S/C19H33ClO4/c1-17(2)13-16-24-19(22)12-11-18(21)23-15-10-8-6-4-3-5-7-9-14
InchiKey: PYXGQSLDEVUUDE-UHFFFAOYSA-N
Formula: C19H33ClO4
SMILES: CC(C)=CCOC(=O)CCC(=O)OCCCCCCCCCCCCI
Mol. weight [g/mol]: 360.92

Physical Properties

Property code	Value	Unit	Source
gf	-299.00	kJ/mol	Joback Method
hf	-833.40	kJ/mol	Joback Method
hfus	53.63	kJ/mol	Joback Method
hvap	80.62	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.179		Crippen Method
mcvol	301.390	ml/mol	McGowan Method
pc	1164.84	kPa	Joback Method
rinpol	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook
tb	828.17	K	Joback Method
tc	1019.01	K	Joback Method
tf	459.09	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.32	J/mol×K	828.17	Joback Method
cpg	930.77	J/mol×K	859.98	Joback Method
cpg	946.26	J/mol×K	891.78	Joback Method
cpg	960.79	J/mol×K	923.59	Joback Method
cpg	974.41	J/mol×K	955.39	Joback Method
cpg	987.14	J/mol×K	987.20	Joback Method
cpg	999.00	J/mol×K	1019.01	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=U390407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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