

Succinic acid, cyclohexylmethyl 10-chlorodecyl ester

Inchi:	InChI=1S/C21H37ClO4/c22-16-10-5-3-1-2-4-6-11-17-25-20(23)14-15-21(24)26-18-19-12
InchiKey:	HTQHYWCGOJKPSM-UHFFFAOYSA-N
Formula:	C21H37ClO4
SMILES:	O=C(CCC(=O)OCC1CCCCC1)OCCCCCCCCCCI
Mol. weight [g/mol]:	388.97

Physical Properties

Property code	Value	Unit	Source
gf	-329.38	kJ/mol	Joback Method
hf	-927.79	kJ/mol	Joback Method
hfus	51.75	kJ/mol	Joback Method
hvap	85.47	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.793		Crippen Method
mcvol	323.010	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	889.44	K	Joback Method
tc	1092.90	K	Joback Method
tf	508.05	K	Joback Method
vc	1.242	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.30	J/molxK	889.44	Joback Method
cpg	1076.05	J/molxK	923.35	Joback Method
cpg	1092.42	J/molxK	957.26	Joback Method
cpg	1107.43	J/molxK	991.17	Joback Method
cpg	1121.12	J/molxK	1025.08	Joback Method
cpg	1133.52	J/molxK	1058.99	Joback Method
cpg	1144.66	J/molxK	1092.90	Joback Method
dvisc	0.0006650	Paxs	508.05	Joback Method

dvisc	0.0003215	Paxs	571.62	Joback Method
dvisc	0.0001798	Paxs	635.18	Joback Method
dvisc	0.0001118	Paxs	698.75	Joback Method
dvisc	0.0000752	Paxs	762.31	Joback Method
dvisc	0.0000538	Paxs	825.88	Joback Method
dvisc	0.0000404	Paxs	889.44	Joback Method

Sources

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=U390413&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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