Succinic acid, cyclohexylmethyl 3-chlorophenyl ester

Inchi: InChI=1S/C17H21ClO4/c18-14-7-4-8-15(11-14)22-17(20)10-9-16(19)21-12-13-5-2-1-3-6-

InchiKey: RQLJLLQTXFWGOJ-UHFFFAOYSA-N

Formula: C17H21ClO4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)OCC1CCCCC1

Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-260.28	kJ/mol	Joback Method
hf	-620.17	kJ/mol	Joback Method
hfus	35.04	kJ/mol	Joback Method
hvap	79.50	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.149		Crippen Method
mcvol	242.890	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	829.58	K	Joback Method
tc	1058.62	K	Joback Method
tf	501.91	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.06	J/mol×K	829.58	Joback Method
cpg	740.53	J/mol×K	867.75	Joback Method
cpg	754.56	J/mol×K	905.93	Joback Method
cpg	767.18	J/mol×K	944.10	Joback Method
cpg	778.43	J/mol×K	982.27	Joback Method
cpg	788.33	J/mol×K	1020.44	Joback Method
cpg	796.90	J/mol×K	1058.62	Joback Method
dvisc	0.0007495	Pa×s	501.91	Joback Method

dvisc	0.0004230	Pa×s	556.52	Joback Method
dvisc	0.0002645	Pa×s	611.13	Joback Method
dvisc	0.0001786	Pa×s	665.75	Joback Method
dvisc	0.0001280	Pa×s	720.36	Joback Method
dvisc	0.0000961	Pa×s	774.97	Joback Method
dvisc	0.0000750	Pa×s	829.58	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=U389854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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