Succinic acid, 2,3-dimethylphenyl isohexyl ester

Inchi: InChI=1S/C18H26O4/c1-13(2)7-6-12-21-17(19)10-11-18(20)22-16-9-5-8-14(3)15(16)4/h5

InchiKey: VHLANOOFCYNUCM-UHFFFAOYSA-N

Formula: C18H26O4

SMILES: Cc1cccc(OC(=O)CCC(=O)OCCCC(C)C)c1C

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-276.45	kJ/mol	Joback Method
hf	-696.14	kJ/mol	Joback Method
hfus	37.69	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.968		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	800.02	K	Joback Method
tc	1002.86	K	Joback Method
tf	473.40	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.07	J/mol×K	800.02	Joback Method
cpg	829.27	J/mol×K	969.06	Joback Method
cpg	817.74	J/mol×K	935.25	Joback Method
cpg	805.16	J/mol×K	901.44	Joback Method
cpg	791.53	J/mol×K	867.63	Joback Method
cpg	776.84	J/mol×K	833.83	Joback Method
cpg	839.79	J/mol×K	1002.86	Joback Method
dvisc	0.0000667	Pa×s	800.02	Joback Method

dvisc	0.0000855	Pa×s	745.58	Joback Method
dvisc	0.0001138	Pa×s	691.15	Joback Method
dvisc	0.0001591	Pa×s	636.71	Joback Method
dvisc	0.0002369	Pa×s	582.27	Joback Method
dvisc	0.0003829	Pa×s	527.84	Joback Method
dvisc	0.0006911	Pa×s	473.40	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=U349622&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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