Succinic acid, 2,3-dimethylphenyl heptyl ester

Inchi: InChI=1S/C19H28O4/c1-4-5-6-7-8-14-22-18(20)12-13-19(21)23-17-11-9-10-15(2)16(17)3
InchiKey: BDAOJSKYRAVJBR-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: CCCCCCCOC(=O)CCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-265.59	kJ/mol	Joback Method
hf	-711.50	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.503		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	2358.00		NIST Webbook
rinpol	2358.00		NIST Webbook
tb	823.34	K	Joback Method
tc	1023.69	K	Joback Method
tf	499.67	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.39	J/mol×K	823.34	Joback Method
cpg	886.82	J/mol×K	990.30	Joback Method
cpg	875.24	J/mol×K	956.91	Joback Method
cpg	862.63	J/mol×K	923.52	Joback Method
cpg	848.96	J/mol×K	890.12	Joback Method
cpg	834.21	J/mol×K	856.73	Joback Method
cpg	897.37	J/mol×K	1023.69	Joback Method
dvisc	0.0000636	Pa×s	823.34	Joback Method

dvisc	0.0000805	Pa×s	769.39	Joback Method
dvisc	0.0001056	Pa×s	715.45	Joback Method
dvisc	0.0001447	Pa×s	661.50	Joback Method
dvisc	0.0002098	Pa×s	607.56	Joback Method
dvisc	0.0003271	Pa×s	553.62	Joback Method
dvisc	0.0005610	Pa×s	499.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U349623&Units=SI

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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