Adipic acid, 2,3-dimethylphenyl octyl ester

Inchi: InChI=1S/C22H34O4/c1-4-5-6-7-8-11-17-25-21(23)15-9-10-16-22(24)26-20-14-12-13-18
InchiKey: SMGGQSAXCRFDSA-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCCCCCCCOC(=O)CCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-240.33	kJ/mol	Joback Method
hf	-773.42	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	86.48	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.673		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2687.00		NIST Webbook
tb	891.98	K	Joback Method
tc	1096.12	K	Joback Method
tf	533.48	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.72	J/mol×K	891.98	Joback Method
cpg	1013.19	J/mol×K	926.00	Joback Method
cpg	1028.42	J/mol×K	960.03	Joback Method
cpg	1042.43	J/mol×K	994.05	Joback Method
cpg	1055.25	J/mol×K	1028.08	Joback Method
cpg	1066.89	J/mol×K	1062.10	Joback Method
cpg	1077.39	J/mol×K	1096.12	Joback Method
dvisc	0.0004177	Pa×s	533.48	Joback Method
dvisc	0.0002348	Pa×s	593.23	Joback Method

dvisc	0.0001467	Pa×s	652.98	Joback Method
dvisc	0.0000992	Pa×s	712.73	Joback Method
dvisc	0.0000712	Pa×s	772.48	Joback Method
dvisc	0.0000537	Pa×s	832.23	Joback Method
dvisc	0.0000420	Pa×s	891.98	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=U353886&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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