Adipic acid, 2,3-dimethylphenyl ethyl ester

Inchi: InChI=1S/C16H22O4/c1-4-19-15(17)10-5-6-11-16(18)20-14-9-7-8-12(2)13(14)3/h7-9H,4-
InchiKey: ABXKNSKJLAOWLH-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCOC(=O)CCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-290.85	kJ/mol	Joback Method
hf	-649.58	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	73.12	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.332		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	2089.00		NIST Webbook
tb	754.70	K	Joback Method
tc	957.28	K	Joback Method
tf	465.86	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.65	J/mol×K	754.70	Joback Method
cpg	713.22	J/mol×K	923.52	Joback Method
cpg	702.00	J/mol×K	889.75	Joback Method
cpg	689.83	J/mol×K	855.99	Joback Method
cpg	676.72	J/mol×K	822.23	Joback Method
cpg	662.66	J/mol×K	788.46	Joback Method
cpg	723.52	J/mol×K	957.28	Joback Method
dvisc	0.0000937	Pa×s	754.70	Joback Method
dvisc	0.0001173	Pa×s	706.56	Joback Method

dvisc	0.0001517	Pa×s	658.42	Joback Method
dvisc	0.0002043	Pa×s	610.28	Joback Method
dvisc	0.0002895	Pa×s	562.14	Joback Method
dvisc	0.0004379	Pa×s	514.00	Joback Method
dvisc	0.0007216	Pa×s	465.86	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=U353878&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