Adipic acid, 2,3-dimethylphenyl propyl ester

Inchi: InChI=1S/C17H24O4/c1-4-12-20-16(18)10-5-6-11-17(19)21-15-9-7-8-13(2)14(15)3/h7-9H
InchiKey: DJUYFHVAOUWDCR-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CCCOC(=O)CCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-282.43	kJ/mol	Joback Method
hf	-670.22	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	75.35	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.722		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	2180.00		NIST Webbook
tb	777.58	K	Joback Method
tc	978.83	K	Joback Method
tf	477.13	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.59	J/mol×K	777.58	Joback Method
cpg	770.30	J/mol×K	945.29	Joback Method
cpg	758.92	J/mol×K	911.75	Joback Method
cpg	746.57	J/mol×K	878.21	Joback Method
cpg	733.23	J/mol×K	844.66	Joback Method
cpg	718.91	J/mol×K	811.12	Joback Method
cpg	780.72	J/mol×K	978.83	Joback Method
dvisc	0.0000827	Pa×s	777.58	Joback Method
dvisc	0.0001039	Pa×s	727.51	Joback Method

dvisc	0.0001350	Pa×s	677.43	Joback Method
dvisc	0.0001829	Pa×s	627.36	Joback Method
dvisc	0.0002612	Pa×s	577.28	Joback Method
dvisc	0.0003993	Pa×s	527.21	Joback Method
dvisc	0.0006671	Pa×s	477.13	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=U353879&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