Adipic acid, di(2,3-dimethylphenyl) ester

Inchi: InChI=1S/C22H26O4/c1-15-9-7-11-19(17(15)3)25-21(23)13-5-6-14-22(24)26-20-12-8-10
InchiKey: HOAZLBPACVBNRI-UHFFFAOYSA-N
Formula: C22H26O4
SMILES: Cc1cccc(OC(=O)CCCCC(=O)Oc2cccc(C)c2C)c1C
Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-147.18	kJ/mol	Joback Method
hf	-559.83	kJ/mol	Joback Method
hfus	44.84	kJ/mol	Joback Method
hvap	90.08	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	4.992		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2862.00		NIST Webbook
tb	928.62	K	Joback Method
tc	1152.72	K	Joback Method
tf	584.94	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.60	J/mol×K	928.62	Joback Method
cpg	908.60	J/mol×K	965.97	Joback Method
cpg	921.22	J/mol×K	1003.32	Joback Method
cpg	932.49	J/mol×K	1040.67	Joback Method
cpg	942.43	J/mol×K	1078.02	Joback Method
cpg	951.07	J/mol×K	1115.37	Joback Method
cpg	958.43	J/mol×K	1152.72	Joback Method
dvisc	0.0002974	Pa×s	584.94	Joback Method
dvisc	0.0001888	Pa×s	642.22	Joback Method

dvisc	0.0001291	Pa×s	699.50	Joback Method
dvisc	0.0000935	Pa×s	756.78	Joback Method
dvisc	0.0000709	Pa×s	814.06	Joback Method
dvisc	0.0000557	Pa×s	871.34	Joback Method
dvisc	0.0000451	Pa×s	928.62	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=U353890&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