

Adipic acid, 2,3-dimethylphenyl pentyl ester

Inchi:	InChI=1S/C19H28O4/c1-4-5-8-14-22-18(20)12-6-7-13-19(21)23-17-11-9-10-15(2)16(17)3
InchiKey:	ZULNEZRKBIFWJJ-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCCCCOC(=O)CCCCC(=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
rinsol	2384.00		NIST Webbook
tb	823.34	K	Joback Method
tc	1023.69	K	Joback Method
tf	499.67	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.39	J/molxK	823.34	Joback Method
cpg	886.82	J/molxK	990.30	Joback Method
cpg	875.24	J/molxK	956.91	Joback Method
cpg	862.63	J/molxK	923.52	Joback Method
cpg	848.96	J/molxK	890.12	Joback Method
cpg	834.21	J/molxK	856.73	Joback Method
cpg	897.37	J/molxK	1023.69	Joback Method
dvisc	0.0000636	Paxs	823.34	Joback Method
dvisc	0.0000805	Paxs	769.39	Joback Method

dvisc	0.0001056	Paxs	715.45	Joback Method
dvisc	0.0001447	Paxs	661.50	Joback Method
dvisc	0.0002098	Paxs	607.56	Joback Method
dvisc	0.0003271	Paxs	553.62	Joback Method
dvisc	0.0005610	Paxs	499.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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