

Adipic acid, 2,3-dimethylphenyl heptyl ester

Inchi:	InChI=1S/C21H32O4/c1-4-5-6-7-10-16-24-20(22)14-8-9-15-21(23)25-19-13-11-12-17(2)
InchiKey:	QCYWQLPRTQWBQA-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	CCCCCCCOC(=O)CCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	348.48

Physical Properties

Property code	Value	Unit	Source
gf	-248.75	kJ/mol	Joback Method
hf	-752.78	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	84.25	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.283		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinsol	2588.00		NIST Webbook
tb	869.10	K	Joback Method
tc	1071.22	K	Joback Method
tf	522.21	K	Joback Method
vc	1.151	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.55	J/molxK	869.10	Joback Method
cpg	952.81	J/molxK	902.79	Joback Method
cpg	967.89	J/molxK	936.47	Joback Method
cpg	981.80	J/molxK	970.16	Joback Method
cpg	994.57	J/molxK	1003.85	Joback Method
cpg	1006.22	J/molxK	1037.54	Joback Method
cpg	1016.76	J/molxK	1071.22	Joback Method
dvisc	0.0004628	Paxs	522.21	Joback Method
dvisc	0.0002633	Paxs	580.02	Joback Method

dvisc	0.0001659	Paxs	637.84	Joback Method
dvisc	0.0001129	Paxs	695.65	Joback Method
dvisc	0.0000815	Paxs	753.47	Joback Method
dvisc	0.0000616	Paxs	811.28	Joback Method
dvisc	0.0000484	Paxs	869.10	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=U353885&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

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