

Adipic acid, 2,3-dimethylphenyl isohexyl ester

Inchi: InChI=1S/C20H30O4/c1-15(2)9-8-14-23-19(21)12-5-6-13-20(22)24-18-11-7-10-16(3)17(4)18
InchiKey: JCURSIBPEAEXOP-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: Cc1cccc(OC(=O)CCCCC(=O)OCCCC(C)C)c1C
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-259.61	kJ/mol	Joback Method
hf	-737.42	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	81.64	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.749		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2443.00		NIST Webbook
rinpol	2443.00		NIST Webbook
tb	845.78	K	Joback Method
tc	1048.38	K	Joback Method
tf	495.94	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.60	J/molxK	845.78	Joback Method
cpg	893.77	J/molxK	879.55	Joback Method
cpg	908.78	J/molxK	913.31	Joback Method
cpg	922.65	J/molxK	947.08	Joback Method
cpg	935.39	J/molxK	980.85	Joback Method
cpg	947.02	J/molxK	1014.62	Joback Method
cpg	957.55	J/molxK	1048.38	Joback Method
dvisc	0.0005710	Paxs	495.94	Joback Method

dvisc	0.0003087	Paxs	554.25	Joback Method
dvisc	0.0001876	Paxs	612.55	Joback Method
dvisc	0.0001244	Paxs	670.86	Joback Method
dvisc	0.0000880	Paxs	729.17	Joback Method
dvisc	0.0000656	Paxs	787.47	Joback Method
dvisc	0.0000509	Paxs	845.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353883&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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