

Adipic acid, nonyl 2,3,5,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C21H28Cl4O4/c1-2-3-4-5-6-7-10-13-28-17(26)11-8-9-12-18(27)29-21-19(24)1
InchiKey:	NSJSVWSXICBEKR-UHFFFAOYSA-N
Formula:	C21H28Cl4O4
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	486.26

Physical Properties

Property code	Value	Unit	Source
gf	-315.73	kJ/mol	Joback Method
hf	-838.68	kJ/mol	Joback Method
hfus	64.99	kJ/mol	Joback Method
hvap	103.12	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	8.060		Crippen Method
mvol	346.830	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	3205.00		NIST Webbook
rinpol	3205.00		NIST Webbook
tb	1028.78	K	Joback Method
tc	1259.68	K	Joback Method
tf	666.93	K	Joback Method
vc	1.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.49	J/molxK	1028.78	Joback Method
cpg	1071.95	J/molxK	1221.20	Joback Method
cpg	1066.14	J/molxK	1182.71	Joback Method
cpg	1059.02	J/molxK	1144.23	Joback Method
cpg	1050.56	J/molxK	1105.75	Joback Method
cpg	1040.72	J/molxK	1067.26	Joback Method
cpg	1076.46	J/molxK	1259.68	Joback Method
dvisc	0.0000261	Paxs	1028.78	Joback Method

dvisc	0.0000323	Paxs	968.47	Joback Method
dvisc	0.0000412	Paxs	908.16	Joback Method
dvisc	0.0000544	Paxs	847.86	Joback Method
dvisc	0.0000749	Paxs	787.55	Joback Method
dvisc	0.0001087	Paxs	727.24	Joback Method
dvisc	0.0001687	Paxs	666.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353954&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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