

Adipic acid, isoheptyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C18H23Cl3O4/c1-12(2)6-5-9-24-16(22)7-3-4-8-17(23)25-13-10-14(19)18(21)15
InchiKey:	MWLCMOQOSODIIT-UHFFFAOYSA-N
Formula:	C18H23Cl3O4
SMILES:	CC(C)CCCOC(=O)CCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]:	409.73

Physical Properties

Property code	Value	Unit	Source
gf	-321.87	kJ/mol	Joback Method
hf	-754.83	kJ/mol	Joback Method
hfus	49.89	kJ/mol	Joback Method
hvap	91.00	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.092		Crippen Method
mvol	292.320	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	917.29	K	Joback Method
tc	1134.50	K	Joback Method
tf	575.68	K	Joback Method
vc	1.125	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.79	J/molxK	917.29	Joback Method
cpg	883.83	J/molxK	1098.30	Joback Method
cpg	876.27	J/molxK	1062.09	Joback Method
cpg	867.60	J/molxK	1025.89	Joback Method
cpg	857.80	J/molxK	989.69	Joback Method
cpg	846.87	J/molxK	953.49	Joback Method
cpg	890.30	J/molxK	1134.50	Joback Method
dvisc	0.0000436	Paxs	917.29	Joback Method

dvisc	0.0000548	Paxs	860.36	Joback Method
dvisc	0.0000711	Paxs	803.42	Joback Method
dvisc	0.0000962	Paxs	746.49	Joback Method
dvisc	0.0001366	Paxs	689.55	Joback Method
dvisc	0.0002067	Paxs	632.62	Joback Method
dvisc	0.0003394	Paxs	575.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353909&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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