Adipic acid, 2,2,2-trichloroethyl undecyl ester

Inchi: InChI=1S/C19H33Cl3O4/c1-2-3-4-5-6-7-8-9-12-15-25-17(23)13-10-11-14-18(24)26-16-19

InchiKey: CBVFROXPBMYZRF-UHFFFAOYSA-N

Formula: C19H33Cl3O4

SMILES: CCCCCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 431.82

Physical Properties

Property code	Value	Unit	Source
gf	-391.69	kJ/mol	Joback Method
hf	-981.06	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	88.06	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.534		Crippen Method
mcvol	330.170	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tb	895.76	K	Joback Method
tc	1098.51	K	Joback Method
tf	540.39	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.08	J/mol×K	895.76	Joback Method
cpg	1013.04	J/mol×K	929.55	Joback Method
cpg	1026.95	J/mol×K	963.34	Joback Method
cpg	1039.83	J/mol×K	997.14	Joback Method
cpg	1051.74	J/mol×K	1030.93	Joback Method
cpg	1062.71	J/mol×K	1064.72	Joback Method
cpg	1072.80	J/mol×K	1098.51	Joback Method
dvisc	0.0004095	Pa×s	540.39	Joback Method

dvisc	0.0002124	Pa×s	599.62	Joback Method
dvisc	0.0001240	Pa×s	658.85	Joback Method
dvisc	0.0000791	Pa×s	718.08	Joback Method
dvisc	0.0000540	Pa×s	777.30	Joback Method
dvisc	0.0000390	Pa×s	836.53	Joback Method
dvisc	0.0000293	Pa×s	895.76	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=U353483&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