Adipic acid, monochloride 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C12H21ClO3/c1-9(12(2,3)4)16-11(15)8-6-5-7-10(13)14/h9H,5-8H2,1-4H3

InchiKey: HYCAONTXXYAGCB-UHFFFAOYSA-N

Formula: C12H21ClO3

SMILES: CC(OC(=O)CCCCC(=O)Cl)C(C)(C)C

Mol. weight [g/mol]: 248.75

Physical Properties

Property code	Value	Unit	Source
gf	-324.21	kJ/mol	Joback Method
hf	-678.16	kJ/mol	Joback Method
hfus	24.48	kJ/mol	Joback Method
hvap	60.91	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.290		Crippen Method
mcvol	201.190	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1557.00		NIST Webbook
tb	637.88	K	Joback Method
tc	832.11	K	Joback Method
tf	364.43	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.95	J/mol×K	637.88	Joback Method
cpg	536.76	J/mol×K	670.25	Joback Method
cpg	550.74	J/mol×K	702.62	Joback Method
cpg	563.92	J/mol×K	734.99	Joback Method
cpg	576.32	J/mol×K	767.36	Joback Method
cpg	587.97	J/mol×K	799.73	Joback Method
cpg	598.91	J/mol×K	832.11	Joback Method
dvisc	0.0027638	Pa×s	364.43	Joback Method
dvisc	0.0012875	Pa×s	410.00	Joback Method

dvisc	0.0006988	Pa×s	455.58	Joback Method
dvisc	0.0004239	Pa×s	501.15	Joback Method
dvisc	0.0002795	Pa×s	546.73	Joback Method
dvisc	0.0001964	Pa×s	592.30	Joback Method
dvisc	0.0001452	Pa×s	637.88	Joback Method

Sources

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=U353685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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