Adipic acid, bis(3,3,5-trimethylhexyl) ester

Other names: Hexanedioic acid, di-(3,3,5-trimethylhexyl) ester
Bis(3,3,5-trimethylhexyl) hexanedioate
Inchi: InChI=1S/C24H46O4/c1-19(2)17-23(5,6)13-15-27-21(25)11-9-10-12-22(26)28-16-14-24(
InchiKey: BVDJZDODWHVXPA-UHFFFAOYSA-N
Formula: C24H46O4
SMILES: CC(C)CC(C)(C)CCOC(=O)CCCCC(=O)OCCC(C)(C)CC(C)C
Mol. weight [g/mol]: 398.62
CAS: 13007-41-5

Physical Properties

Property code	Value	Unit	Source
gf	-315.84	kJ/mol	Joback Method
hf	-1056.35	kJ/mol	Joback Method
hfus	41.62	kJ/mol	Joback Method
hvap	83.96	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	6.558		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
tb	893.76	K	Joback Method
tc	1095.04	K	Joback Method
tf	479.40	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.60	J/mol×K	893.76	Joback Method
cpg	1238.26	J/mol×K	927.31	Joback Method
cpg	1256.64	J/mol×K	960.85	Joback Method
cpg	1273.81	J/mol×K	994.40	Joback Method
cpg	1289.83	J/mol×K	1027.95	Joback Method
cpg	1304.78	J/mol×K	1061.50	Joback Method
cpg	1318.71	J/mol×K	1095.04	Joback Method

dvisc	0.0006231	Pa×s	479.40	Joback Method
dvisc	0.0002259	Pa×s	548.46	Joback Method
dvisc	0.0001027	Pa×s	617.52	Joback Method
dvisc	0.0000548	Pa×s	686.58	Joback Method
dvisc	0.0000327	Pa×s	755.64	Joback Method
dvisc	0.0000213	Pa×s	824.70	Joback Method
dvisc	0.0000149	Pa×s	893.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C13007415&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume