Adipic acid, 3-oxobut-2-yl tridecyl ester

Inchi: InChI=1S/C23H42O5/c1-4-5-6-7-8-9-10-11-12-13-16-19-27-22(25)17-14-15-18-23(26)28
InchiKey: JSAAKZPEPQMEII-UHFFFAOYSA-N
Formula: C23H42O5
SMILES: CCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 398.58

Physical Properties

Property code	Value	Unit	Source
gf	-456.42	kJ/mol	Joback Method
hf	-1125.51	kJ/mol	Joback Method
hfus	58.98	kJ/mol	Joback Method
hvap	91.46	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.922		Crippen Method
mcvol	351.380	ml/mol	McGowan Method
pc	939.22	kPa	Joback Method
rinpol	2724.00		NIST Webbook
tb	931.65	K	Joback Method
tc	1141.56	K	Joback Method
tf	528.22	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.67	J/mol×K	931.65	Joback Method
cpg	1194.68	J/mol×K	966.64	Joback Method
cpg	1211.25	J/mol×K	1001.62	Joback Method
cpg	1226.41	J/mol×K	1036.61	Joback Method
cpg	1240.19	J/mol×K	1071.59	Joback Method
cpg	1252.63	J/mol×K	1106.58	Joback Method
cpg	1263.75	J/mol×K	1141.56	Joback Method
dvisc	0.0005155	Pa×s	528.22	Joback Method
dvisc	0.0002441	Pa×s	595.46	Joback Method

dvisc	0.0001345	Pa×s	662.70	Joback Method
dvisc	0.0000828	Pa×s	729.93	Joback Method
dvisc	0.0000552	Pa×s	797.17	Joback Method
dvisc	0.0000393	Pa×s	864.41	Joback Method
dvisc	0.0000293	Pa×s	931.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353757&Units=SI
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

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