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

Inchi: InChI=1S/C24H44O5/c1-4-5-6-7-8-9-10-11-12-13-14-17-20-28-23(26)18-15-16-19-24(27
InchiKey: SQIDMGKABCMSCM-UHFFFAOYSA-N
Formula: C24H44O5
SMILES: CCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 412.60

Physical Properties

Property code	Value	Unit	Source
gf	-448.00	kJ/mol	Joback Method
hf	-1146.15	kJ/mol	Joback Method
hfus	61.57	kJ/mol	Joback Method
hvap	93.69	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	6.312		Crippen Method
mcvol	365.470	ml/mol	McGowan Method
pc	886.30	kPa	Joback Method
rinpol	2824.00		NIST Webbook
tb	954.53	K	Joback Method
tc	1171.53	K	Joback Method
tf	539.49	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.17	J/mol×K	954.53	Joback Method
cpg	1316.12	J/mol×K	1135.36	Joback Method
cpg	1303.71	J/mol×K	1099.20	Joback Method
cpg	1289.85	J/mol×K	1063.03	Joback Method
cpg	1274.50	J/mol×K	1026.86	Joback Method
cpg	1257.62	J/mol×K	990.70	Joback Method
cpg	1327.12	J/mol×K	1171.53	Joback Method
dvisc	0.0000251	Pa×s	954.53	Joback Method
dvisc	0.0000337	Pa×s	885.36	Joback Method

dvisc	0.0000475	Pa×s	816.18	Joback Method
dvisc	0.0000714	Pa×s	747.01	Joback Method
dvisc	0.0001166	Pa×s	677.84	Joback Method
dvisc	0.0002128	Pa×s	608.66	Joback Method
dvisc	0.0004535	Pa×s	539.49	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=U353758&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