Sebacic acid, 3-oxobut-2-yl undecyl ester

Inchi: InChI=1S/C25H46O5/c1-4-5-6-7-8-9-12-15-18-21-29-24(27)19-16-13-10-11-14-17-20-25
InchiKey: CAJIULZBBWDSDY-UHFFFAOYSA-N
Formula: C25H46O5
SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 426.63

Physical Properties

Property code	Value	Unit	Source
gf	-439.58	kJ/mol	Joback Method
hf	-1166.79	kJ/mol	Joback Method
hfus	64.16	kJ/mol	Joback Method
hvap	95.91	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.702		Crippen Method
mcvol	379.560	ml/mol	McGowan Method
pc	837.73	kPa	Joback Method
rinpol	2957.00		NIST Webbook
tb	977.41	K	Joback Method
tc	1202.65	K	Joback Method
tf	550.76	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1302.11	J/mol×K	977.41	Joback Method
cpg	1321.02	J/mol×K	1014.95	Joback Method
cpg	1338.22	J/mol×K	1052.49	Joback Method
cpg	1353.76	J/mol×K	1090.03	Joback Method
cpg	1367.67	J/mol×K	1127.57	Joback Method
cpg	1380.02	J/mol×K	1165.11	Joback Method
cpg	1390.84	J/mol×K	1202.65	Joback Method
dvisc	0.0003979	Pa×s	550.76	Joback Method
dvisc	0.0001851	Pa×s	621.87	Joback Method

dvisc	0.0001008	Pa×s	692.98	Joback Method
dvisc	0.0000614	Pa×s	764.09	Joback Method
dvisc	0.0000408	Pa×s	835.19	Joback Method
dvisc	0.0000288	Pa×s	906.30	Joback Method
dvisc	0.0000214	Pa×s	977.41	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=U355783&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