Glutaric acid, 3-methylbut-2-enyl undecyl ester

Inchi: InChI=1S/C21H38O4/c1-4-5-6-7-8-9-10-11-12-17-24-20(22)14-13-15-21(23)25-18-16-19
InchiKey: KQQBXJRXHGGVDO-UHFFFAOYSA-N
Formula: C21H38O4
SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-270.23	kJ/mol	Joback Method
hf	-858.94	kJ/mol	Joback Method
hfus	54.61	kJ/mol	Joback Method
hvap	80.69	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.740		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1050.73	kPa	Joback Method
rinpol	2512.00		NIST Webbook
tb	836.50	K	Joback Method
tc	1026.26	K	Joback Method
tf	451.71	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.08	J/mol×K	836.50	Joback Method
cpg	1022.24	J/mol×K	868.13	Joback Method
cpg	1039.35	J/mol×K	899.75	Joback Method
cpg	1055.42	J/mol×K	931.38	Joback Method
cpg	1070.51	J/mol×K	963.01	Joback Method
cpg	1084.62	J/mol×K	994.64	Joback Method
cpg	1097.81	J/mol×K	1026.26	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=U360095&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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