Glutaric acid, octyl pent-4-enyl ester

Inchi: InChI=1S/C18H32O4/c1-3-5-7-8-9-11-16-22-18(20)14-12-13-17(19)21-15-10-6-4-2/h4H,2
InchiKey: PPUZSTJXIPHYRX-UHFFFAOYSA-N
Formula: C18H32O4
SMILES: C=CCCCOC(=O)CCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-279.32	kJ/mol	Joback Method
hf	-779.02	kJ/mol	Joback Method
hfus	46.67	kJ/mol	Joback Method
hvap	73.30	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.570		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
rinpol	2191.00		NIST Webbook
tb	760.50	K	Joback Method
tc	940.16	K	Joback Method
tf	435.18	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.69	J/mol×K	760.50	Joback Method
cpg	899.29	J/mol×K	910.22	Joback Method
cpg	885.90	J/mol×K	880.27	Joback Method
cpg	871.66	J/mol×K	850.33	Joback Method
cpg	856.55	J/mol×K	820.39	Joback Method
cpg	840.57	J/mol×K	790.44	Joback Method
cpg	911.85	J/mol×K	940.16	Joback Method
dvisc	0.0000751	Pa×s	760.50	Joback Method
dvisc	0.0000984	Pa×s	706.28	Joback Method

dvisc	0.0001348	Pa×s	652.06	Joback Method
dvisc	0.0001956	Pa×s	597.84	Joback Method
dvisc	0.0003058	Pa×s	543.62	Joback Method
dvisc	0.0005276	Pa×s	489.40	Joback Method
dvisc	0.0010429	Pa×s	435.18	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=U359987&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