Glutaric acid, 3,4-dimethylphenyl pentyl ester

Inchi: InChI=1S/C18H26O4/c1-4-5-6-12-21-17(19)8-7-9-18(20)22-16-11-10-14(2)15(3)13-16/h1
InchiKey: UTJCXXYOXQXCKC-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CCCCCOC(=O)CCCC(=O)Oc1ccc(C)c(C)c1
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-274.01	kJ/mol	Joback Method
hf	-690.86	kJ/mol	Joback Method
hfus	41.21	kJ/mol	Joback Method
hvap	77.57	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.113		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	2367.00		NIST Webbook
tb	800.46	K	Joback Method
tc	1000.95	K	Joback Method
tf	488.40	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.53	J/mol×K	800.46	Joback Method
cpg	828.18	J/mol×K	967.54	Joback Method
cpg	816.68	J/mol×K	934.12	Joback Method
cpg	804.18	J/mol×K	900.71	Joback Method
cpg	790.66	J/mol×K	867.29	Joback Method
cpg	776.12	J/mol×K	833.88	Joback Method
cpg	838.68	J/mol×K	1000.95	Joback Method
dvisc	0.0000726	Pa×s	800.46	Joback Method
dvisc	0.0000916	Pa×s	748.45	Joback Method

dvisc	0.0001196	Pa×s	696.44	Joback Method
dvisc	0.0001630	Pa×s	644.43	Joback Method
dvisc	0.0002346	Pa×s	592.42	Joback Method
dvisc	0.0003622	Pa×s	540.41	Joback Method
dvisc	0.0006133	Pa×s	488.40	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=U359180&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