Glutaric acid, 2,5-dimethylphenyl isohexyl ester

Inchi: InChI=1S/C19H28O4/c1-14(2)7-6-12-22-18(20)8-5-9-19(21)23-17-13-15(3)10-11-16(17)4

InchiKey: CRGDPPKAHAKTIM-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: Cc1ccc(C)c(OC(=O)CCCC(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-268.03	kJ/mol	Joback Method
hf	-716.78	kJ/mol	Joback Method
hfus	40.28	kJ/mol	Joback Method
hvap	79.41	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.359		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	2340.00		NIST Webbook
tb	822.90	K	Joback Method
tc	1025.30	K	Joback Method
tf	484.67	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.92	J/mol×K	822.90	Joback Method
cpg	834.90	J/mol×K	856.63	Joback Method
cpg	849.76	J/mol×K	890.37	Joback Method
cpg	863.52	J/mol×K	924.10	Joback Method
cpg	876.19	J/mol×K	957.83	Joback Method
cpg	887.79	J/mol×K	991.56	Joback Method
cpg	898.33	J/mol×K	1025.30	Joback Method
dvisc	0.0006296	Pa×s	484.67	Joback Method
dvisc	0.0003445	Pa×s	541.04	Joback Method

dvisc	0.0002112	Pa×s	597.41	Joback Method
dvisc	0.0001409	Pa×s	653.78	Joback Method
dvisc	0.0001002	Pa×s	710.16	Joback Method
dvisc	0.0000750	Pa×s	766.53	Joback Method
dvisc	0.0000584	Pa×s	822.90	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=U358939&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