Glutaric acid, hept-2-yl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C20H30O4/c1-5-6-7-11-16(3)23-19(21)13-9-14-20(22)24-18-12-8-10-15(2)17(1

InchiKey: JKCLYBKAUABPGW-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: CCCCCC(C)OC(=O)CCCC(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-259.61	kJ/mol	Joback Method
hf	-737.42	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	81.64	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.891		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2373.00		NIST Webbook
rinpol	2373.00		NIST Webbook
tb	845.78	K	Joback Method
tc	1048.38	K	Joback Method
tf	495.94	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.60	J/mol×K	845.78	Joback Method
cpg	893.77	J/mol×K	879.55	Joback Method
cpg	908.78	J/mol×K	913.31	Joback Method
cpg	922.65	J/mol×K	947.08	Joback Method
cpg	935.39	J/mol×K	980.85	Joback Method
cpg	947.02	J/mol×K	1014.62	Joback Method
cpg	957.55	J/mol×K	1048.38	Joback Method
dvisc	0.0005710	Pa×s	495.94	Joback Method

dvisc	0.0003087	Pa×s	554.25	Joback Method
dvisc	0.0001876	Pa×s	612.55	Joback Method
dvisc	0.0001244	Pa×s	670.86	Joback Method
dvisc	0.0000880	Pa×s	729.17	Joback Method
dvisc	0.0000656	Pa×s	787.47	Joback Method
dvisc	0.0000509	Pa×s	845.78	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=U392220&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