Glutaric acid, cyclohexylmethyl 2-ethylphenyl ester

Inchi: InChI=1S/C20H28O4/c1-2-17-11-6-7-12-18(17)24-20(22)14-8-13-19(21)23-15-16-9-4-3-5

InchiKey: WQXDSPOMGQPOFL-UHFFFAOYSA-N

Formula: C20H28O4

SMILES: CCc1ccccc1OC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-223.09	kJ/mol	Joback Method
hf	-666.35	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	81.79	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.448		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	860.79	K	Joback Method
tc	1080.02	K	Joback Method
tf	505.80	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.90	J/mol×K	860.79	Joback Method
cpg	889.87	J/mol×K	897.33	Joback Method
cpg	905.35	J/mol×K	933.87	Joback Method
cpg	919.38	J/mol×K	970.41	Joback Method
cpg	931.98	J/mol×K	1006.95	Joback Method
cpg	943.20	J/mol×K	1043.49	Joback Method
cpg	953.07	J/mol×K	1080.02	Joback Method
dvisc	0.0006749	Pa×s	505.80	Joback Method

dvisc	0.0003599	Pa×s	564.97	Joback Method
dvisc	0.0002162	Pa×s	624.13	Joback Method
dvisc	0.0001419	Pa×s	683.29	Joback Method
dvisc	0.0000996	Pa×s	742.46	Joback Method
dvisc	0.0000736	Pa×s	801.62	Joback Method
dvisc	0.0000568	Pa×s	860.79	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=U391828&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

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