Glutaric acid, 2-ethylhexyl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C21H32O5/c1-5-7-9-17(6-2)15-25-20(22)10-8-11-21(23)26-19-14-16(3)12-13-1

InchiKey: YRMOQCAQVBXMGZ-UHFFFAOYSA-N

Formula: C21H32O5

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-356.19	kJ/mol	Joback Method
hf	-890.28	kJ/mol	Joback Method
hfus	46.65	kJ/mol	Joback Method
hvap	86.27	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.839		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2565.00		NIST Webbook
rinpol	2565.00		NIST Webbook
tb	891.08	K	Joback Method
tc	1096.53	K	Joback Method
tf	529.44	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.54	J/mol×K	891.08	Joback Method
cpg	1032.40	J/mol×K	1062.29	Joback Method
cpg	1021.83	J/mol×K	1028.05	Joback Method
cpg	1009.97	J/mol×K	993.81	Joback Method
cpg	996.80	J/mol×K	959.56	Joback Method
cpg	982.33	J/mol×K	925.32	Joback Method
cpg	1041.68	J/mol×K	1096.53	Joback Method
dvisc	0.0000331	Pa×s	891.08	Joback Method

dvisc	0.0000426	Pa×s	830.81	Joback Method
dvisc	0.0000572	Pa×s	770.53	Joback Method
dvisc	0.0000806	Pa×s	710.26	Joback Method
dvisc	0.0001210	Pa×s	649.99	Joback Method
dvisc	0.0001975	Pa×s	589.71	Joback Method
dvisc	0.0003603	Pa×s	529.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U393927&Units=SI

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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