Glutaric acid, 2-ethylhexyl 4-acetylphenyl ester

Inchi: InChI=1S/C21H30O5/c1-4-6-8-17(5-2)15-25-20(23)9-7-10-21(24)26-19-13-11-18(12-14-1

InchiKey: PHYGVXYMVQJHQW-UHFFFAOYSA-N

Formula: C21H30O5

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1

Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-370.48	kJ/mol	Joback Method
hf	-859.17	kJ/mol	Joback Method
hfus	47.45	kJ/mol	Joback Method
hvap	89.95	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.724		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2732.00		NIST Webbook
rinpol	2732.00		NIST Webbook
tb	917.55	K	Joback Method
tc	1128.93	K	Joback Method
tf	544.62	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.73	J/mol×K	917.55	Joback Method
cpg	968.28	J/mol×K	952.78	Joback Method
cpg	981.54	J/mol×K	988.01	Joback Method
cpg	993.55	J/mol×K	1023.24	Joback Method
cpg	1004.33	J/mol×K	1058.47	Joback Method
cpg	1013.91	J/mol×K	1093.70	Joback Method
cpg	1022.32	J/mol×K	1128.93	Joback Method
dvisc	0.0004831	Pa×s	544.62	Joback Method

dvisc	0.0002602	Pa×s	606.77	Joback Method
dvisc	0.0001572	Pa×s	668.93	Joback Method
dvisc	0.0001035	Pa×s	731.09	Joback Method
dvisc	0.0000727	Pa×s	793.24	Joback Method
dvisc	0.0000538	Pa×s	855.39	Joback Method
dvisc	0.0000415	Pa×s	917.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392035&Units=SI
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

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