Glutaric acid, 2-ethylhexyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C26H34O5/c1-3-5-11-21(4-2)19-29-25(27)16-10-17-26(28)30-20-22-12-9-15-2

InchiKey: PJYHRMMNGOOHRG-UHFFFAOYSA-N

Formula: C26H34O5

SMILES: CCCCC(CC)COC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 426.55

Physical Properties

Property code	Value	Unit	Source
gf	-192.05	kJ/mol	Joback Method
hf	-745.48	kJ/mol	Joback Method
hfus	54.03	kJ/mol	Joback Method
hvap	99.02	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.452		Crippen Method
mcvol	350.430	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	3136.00		NIST Webbook
rinpol	3136.00		NIST Webbook
tb	1027.18	K	Joback Method
tc	1258.50	K	Joback Method
tf	599.69	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.20	J/mol×K	1027.18	Joback Method
cpg	1216.11	J/mol×K	1219.94	Joback Method
cpg	1209.10	J/mol×K	1181.39	Joback Method
cpg	1200.56	J/mol×K	1142.84	Joback Method
cpg	1190.43	J/mol×K	1104.29	Joback Method
cpg	1178.66	J/mol×K	1065.73	Joback Method
cpg	1221.62	J/mol×K	1258.50	Joback Method
dvisc	0.0000158	Pa×s	1027.18	Joback Method

dvisc	0.0000206	Pa×s	955.93	Joback Method
dvisc	0.0000281	Pa×s	884.68	Joback Method
dvisc	0.0000404	Pa×s	813.43	Joback Method
dvisc	0.0000624	Pa×s	742.19	Joback Method
dvisc	0.0001054	Pa×s	670.94	Joback Method
dvisc	0.0002020	Pa×s	599.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392129&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

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