Glutaric acid, isobutyl 2-phenoxyethyl ester

Inchi: InChI=1S/C17H24O5/c1-14(2)13-22-17(19)10-6-9-16(18)21-12-11-20-15-7-4-3-5-8-15/h3
InchiKey: JRCVQXGJIUQWAG-UHFFFAOYSA-N
Formula: C17H24O5
SMILES: CC(C)COC(=O)CCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-370.61	kJ/mol	Joback Method
hf	-784.78	kJ/mol	Joback Method
hfus	37.07	kJ/mol	Joback Method
hvap	76.05	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.978		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	2253.00		NIST Webbook
rinpol	2253.00		NIST Webbook
tb	789.60	K	Joback Method
tc	991.44	K	Joback Method
tf	459.32	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.03	J/mol×K	789.60	Joback Method
cpg	799.66	J/mol×K	957.80	Joback Method
cpg	788.68	J/mol×K	924.16	Joback Method
cpg	776.64	J/mol×K	890.52	Joback Method
cpg	763.52	J/mol×K	856.88	Joback Method
cpg	749.32	J/mol×K	823.24	Joback Method
cpg	809.57	J/mol×K	991.44	Joback Method
dvisc	0.0000569	Pa×s	789.60	Joback Method

dvisc	0.0000746	Pa×s	734.55	Joback Method
dvisc	0.0001020	Pa×s	679.51	Joback Method
dvisc	0.0001474	Pa×s	624.46	Joback Method
dvisc	0.0002289	Pa×s	569.41	Joback Method
dvisc	0.0003904	Pa×s	514.37	Joback Method
dvisc	0.0007568	Pa×s	459.32	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=U376914&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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