

Fumaric acid, 4-phenoxybenzyl undecyl ester

Inchi: InChI=1S/C28H36O5/c1-2-3-4-5-6-7-8-9-13-22-31-27(29)20-21-28(30)32-23-24-16-18-26
InchiKey: XGCKOFXLMNEWMM-QZQOTICOSA-N
Formula: C28H36O5
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 452.58

Physical Properties

Property code	Value	Unit	Source
gf	-92.55	kJ/mol	Joback Method
hf	-664.26	kJ/mol	Joback Method
hfus	62.93	kJ/mol	Joback Method
hvap	103.82	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.152		Crippen Method
mcvol	374.310	ml/mol	McGowan Method
pc	1019.43	kPa	Joback Method
rinpol	3504.00		NIST Webbook
tb	1077.54	K	Joback Method
tc	1319.33	K	Joback Method
tf	632.15	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.82	J/molxK	1077.54	Joback Method
cpg	1271.47	J/molxK	1117.84	Joback Method
cpg	1283.51	J/molxK	1158.14	Joback Method
cpg	1294.03	J/molxK	1198.43	Joback Method
cpg	1303.12	J/molxK	1238.73	Joback Method
cpg	1310.85	J/molxK	1279.03	Joback Method
cpg	1317.32	J/molxK	1319.33	Joback Method
dvisc	0.0001348	Paxs	632.15	Joback Method
dvisc	0.0000717	Paxs	706.38	Joback Method

dvisc	0.0000430	Paxs	780.61	Joback Method
dvisc	0.0000282	Paxs	854.85	Joback Method
dvisc	0.0000198	Paxs	929.08	Joback Method
dvisc	0.0000146	Paxs	1003.31	Joback Method
dvisc	0.0000113	Paxs	1077.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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