Sebacic acid, butyl 2-methylbenzyl ester

Inchi: InChI=1S/C22H34O4/c1-3-4-17-25-21(23)15-9-7-5-6-8-10-16-22(24)26-18-20-14-12-11-1
InchiKey: XZWBPENQQYSPMJ-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1C
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-230.70	kJ/mol	Joback Method
hf	-761.95	kJ/mol	Joback Method
hfus	51.96	kJ/mol	Joback Method
hvap	85.82	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.502		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2672.00		NIST Webbook
rinpol	2672.00		NIST Webbook
tb	887.00	K	Joback Method
tc	1090.20	K	Joback Method
tf	520.96	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.29	J/mol×K	887.00	Joback Method
cpg	1013.85	J/mol×K	920.87	Joback Method
cpg	1029.18	J/mol×K	954.73	Joback Method
cpg	1043.31	J/mol×K	988.60	Joback Method
cpg	1056.27	J/mol×K	1022.47	Joback Method
cpg	1068.08	J/mol×K	1056.33	Joback Method
cpg	1078.77	J/mol×K	1090.20	Joback Method
dvisc	0.0004813	Pa×s	520.96	Joback Method

dvisc	0.0002579	Pa×s	581.97	Joback Method
dvisc	0.0001556	Pa×s	642.97	Joback Method
dvisc	0.0001024	Pa×s	703.98	Joback Method
dvisc	0.0000721	Pa×s	764.99	Joback Method
dvisc	0.0000534	Pa×s	825.99	Joback Method
dvisc	0.0000413	Pa×s	887.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380715&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

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