Glutaric acid, 2-bromobenzyl tetradecyl ester

Inchi: InChI=1S/C26H41BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-15-21-30-25(28)19-16-20-26(29)31-
InchiKey: ZSRAECVKZZPJGX-UHFFFAOYSA-N
Formula: C26H41BrO4
SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccccc1Br
Mol. weight [g/mol]: 497.50

Physical Properties

Property code	Value	Unit	Source
gf	-182.70	kJ/mol	Joback Method
hf	-818.18	kJ/mol	Joback Method
hfus	67.61	kJ/mol	Joback Method
hvap	101.15	kJ/mol	Joback Method
log10ws	-9.19		Crippen Method
logp	7.907		Crippen Method
mcvol	385.820	ml/mol	McGowan Method
pc	954.37	kPa	Joback Method
rinpol	3398.00		NIST Webbook
rinpol	3398.00		NIST Webbook
tb	1044.68	K	Joback Method
tc	1281.15	K	Joback Method
tf	625.84	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.30	J/mol×K	1044.68	Joback Method
cpg	1299.27	J/mol×K	1084.09	Joback Method
cpg	1313.68	J/mol×K	1123.50	Joback Method
cpg	1326.62	J/mol×K	1162.92	Joback Method
cpg	1338.15	J/mol×K	1202.33	Joback Method
cpg	1348.36	J/mol×K	1241.74	Joback Method
cpg	1357.32	J/mol×K	1281.15	Joback Method
dvisc	0.0001884	Pa×s	625.84	Joback Method

dvisc	0.0001030	Pa×s	695.65	Joback Method
dvisc	0.0000629	Pa×s	765.45	Joback Method
dvisc	0.0000417	Pa×s	835.26	Joback Method
dvisc	0.0000295	Pa×s	905.07	Joback Method
dvisc	0.0000219	Pa×s	974.87	Joback Method
dvisc	0.0000169	Pa×s	1044.68	Joback Method

Sources

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=U376772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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